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ALOHA Computer Code Application Guidance for Documented Safety Analysis

Interim Report

U.S. Department of Energy

Office of Environment, Safety and Health

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FOREWORD

This document provides guidance to Department of Energy (DOE) facility analysts in the use of the ALOHA computer code for supporting Documented Safety Analysis applications. Information is provided herein that supplements information found in the ALOHA documentation provided by the code developer. ALOHA is one of six computer codes designated by DOE's Office of Environmental, Safety and Health as a toolbox code for safety analysis.

Suggestions for corrections or improvements to this document should be addressed to –

Chip Lagdon
EH-31/GTN
Office of Quality Assurance Programs
U.S. Department of Energy
Washington, D.C. 20585-2040
Phone (301) 903-4218
Email: Chip.Lagdon@hq.doe.gov

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EXECUTIVE SUMMARY

The Defense Nuclear Facilities Safety Board issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002. The Recommendation identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, Software Quality Assurance (SQA)-compliant safety analysis codes is one of the major commitments contained in the February 28, 2003 *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*. In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications (DOE, 2002b). The Areal Locations of Hazardous Atmospheres (ALOHA) code, is one of the designated toolbox codes.

ALOHA may require some degree of quality assurance improvement before meeting current SQA standards. In the interim period before these changes are completed, ALOHA is considered a useful asset in the support of safety basis calculations. To ensure appropriate application of the designated toolbox software, the Implementation Plan has committed to sponsoring a set of code-specific documents to guide informed use of the software, and supplement the available user's manual information.

The ALOHA guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

Use of the information contained here, although not ensuring correct use of ALOHA in each analytical context will minimize potential user errors and the likelihood of ALOHA use outside its regime of applicability.

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1.0 INTRODUCTION

In January 2000, the Defense Nuclear Facilities Safety Board (DNFSB) issued Technical Report 25, (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2000). TECH-25 identified issues regarding the state of software quality assurance (SQA) in the Department of Energy (DOE) Complex for software used to make safety analysis decisions and to control safety-related systems. Instances were noted in which computer codes were either inappropriately applied or were executed with incorrect input data. Of particular concern were inconsistencies in the exercise of SQA from site to site, and from facility to facility, and the variability in guidance and training in the appropriate use of accident analysis software.

During the subsequent 2000 to 2002 period, survey information on SQA programs, processes, and procedures was collected as well as the initial elements to a response plan. However, to expedite implementation of corrective actions in this area, the DNFSB issued Recommendation 2002-1, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2002). As part of its Recommendation to the DOE, the DNFSB enumerated many of the points noted earlier in TECH-25, but noted specific concerns regarding the quality of the software used to analyze and guide safety-related decisions, the quality of the software used to design or develop safety-related controls, and the proficiency of personnel using the software.

DOE has developed a series of actions that address the Board's concerns, contained in the Implementation Plan for the DNFSB Recommendation, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1.* Two of the actions include:

(i) identification of a set of accident analysis software that is widely used in the DOE Complex, and

(ii) issuance of code-specific guidance reports on the use of the "toolbox" codes for DOE facility accident analysis, identifying applicable regime in accident analysis, default inputs, and special conditions for use.

Safety analysis software for the DOE "toolbox" status was designated by the DOE Office of Environment, Safety and Health (DOE/EH, 2003). The supporting basis for this designation was provided by a DOE-chartered Safety Analysis Software Group in a technical report entitled, *Selection of Computer Codes for DOE Safety Analysis Applications*, (http://www.deprep.org/archive/rec/2002-1/NNSACCodes1.pdf), and includes version 5.2.3 of the Areal Locations of Hazardous Atmospheres (ALOHA) code.

It is believed that each code designated for the toolbox can be applied to accident analysis under the precautions and recommended input parameter ranges documented in the body of this report. The code-specific document will be maintained and updated until a minimum qualification software package is completed.

The contents of this report are applicable in the interim period until measures are completed to bring ALOHA into compliance with defined SQA standards. The primary objective of the guidance report is to provide information on the use of ALOHA for supporting DOE safety basis accident analysis. Specifically, the report contains:

- Applicability guidance for Documented Safety Analysis (DSA)-type analysis, specifically tailored for DOE safety analysis
- Appropriate regimes, recommended configurations
- Overcoming known vulnerabilities and avoiding code errors
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications
- Default input value recommendations for site-independent parameters, and
- Citations of currently available SQA documentation.

Thus, this report is intended to complement existing ALOHA user's documentation. The latter tend to be much broader in coverage of the full range of capabilities of ALOHA and the spectrum of inputs that might be needed depending upon the application, but lack cohesive and targeted guidance for particular applications such as DSA accident analyses. Furthermore, the goal of this document is to identify limitations and vulnerabilities not readily found in documentation from the code developer or published elsewhere.

The ALOHA guidance document is written using the following set of sections. The first section contains an introduction and background providing an overview of toolbox software in the context of 10 CFR 830 (CFR, 2001). More information follows on the scope and purpose of this document. The next major section is a summary description of ALOHA. A third section discusses applicable regimes for using ALOHA in performing accident analysis. A large section on default inputs and recommendations, emphasizing appropriate inputs for DOE applications, succeeds this section. Following this discussion are sections on special conditions for use of the software and software limitations. A sample case is then provided, followed by acronyms and definitions, references, and appendices.

1.1 Background: Overview of Toolbox Software in Context of 10 CFR 830

In the context of 10 CFR 830, the Nuclear Safety Management rule, the six computer codes designated by DOE/EH as toolbox software, will be of appropriate pedigree for support of safety basis documentation. After completion of the minimum required SQA upgrade measures for a toolbox code, the safety analyst would still need to justify the specific application with the code of interest, input parameters, and user assumptions, but many SQA burdens would be reduced from current requirements. The user would need to reference the toolbox code and version, identify compliance with their organization's SQA requirements and demonstrate that the code is being applied in the proper accident analysis context using appropriate inputs. The SQA pedigree would be sufficiently established for technical review purposes since the code is recognized as toolbox-supported.

Only six codes out of more than one hundred software packages applied in the DOE Complex for accident analysis purpose have been designated as "toolbox" codes (DOE, 2002b). Other non-toolbox, dispersion and consequence software can still be applied in the context of support safety basis applications. However, each organization applying this category of software will need to demonstrate compliance with applicable SQA criteria, such as those applied to the toolbox software.

1.2 Scope

The ALOHA guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

1.3 Purpose

The Areal Locations of Hazardous Atmospheres (ALOHA) code, while part of the toolbox collection of software, still may require Software Quality Assurance (SQA) upgrades prior to meeting current established standards for software. However, until these ALOHA upgrades are completed so that ALOHA meets current established standards for software, ALOHA can be applied safety under the condition that the guidance contained in this report is followed. Once upgrades are finalized with ALOHA, it will be brought under configuration control and placed in the toolbox.

Use of the information contained here, although not ensuring correct use of ALOHA in all analytical contexts, will minimize potential user errors and the likelihood of use outside regimes of applicability.

1.4 Applicability

It is recognized that other computer codes besides ALOHA exist that perform similar type of source term and downwind concentration calculations. Moreover, manual or electronic spreadsheet calculations can be a viable alternative to using a computer code for many accident analysis applications that involve chemical spills. The relative merits of using a different computer program or using a hand calculation for a given application is a judgment that must be made by the analyst on a case-by-case basis.

The U.S. Department of Energy (DOE) has provided guidance and general recommendations in this area through the Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program. As part of this program, the chemical dispersion and consequence assessment (CDCA) Working Group (WG) was established to address issues and evaluate methodologies in the CDCA domain. Other WGs were also established for other domains of safety analysis (i.e., fire analysis, explosion analysis, spill source term analysis, in-facility transport analysis, and radiological dispersion and consequence assessment). The CDCA WG (also referred to as WG 6) issued a report that identifies and evaluates methodologies and computer codes to support CDCA applications (Lazaro, 1997). Also of interest is the WG 3 report, which performed a similar function for source term analysis of spills (Brereton, 1997).

The CDCA WG 6 report identified the ALOHA computer code as a recommended code that is "applicable to generally broad safety basis documentation applications." The ALOHA code was similarly recommended by the Spills WG 3 report. In addition to code recommendations, both the Spills WG 3 report and the CDCA WG 6 report also provide a broad set of recommended "best practices" for modeling chemical releases to the atmosphere.

This report builds upon the WG 3 and WG 6 work to provide guidance and recommendations that are targeted to the use of the ALOHA code to calculate source terms and downwind concentrations.

2.0 SUMMARY DESCRIPTION OF THE ALOHA CODE

This section provides a summary form description of the ALOHA. A brief overview is given with additional information to follow in other sections and appendices of the report to provide more in-depth coverage of topics such as the principles of source term development for analysis of accidents that involve chemical inventories, the interface with dispersion conditions in the atmosphere, and the overall assessment of toxicological exposure to receptors.

2.1 ALOHA Code Development

The current version (as of September 2002) of the Areal Locations of Hazardous Atmospheres (ALOHA) code is version 5.2.3, was released in 1999. ALOHA is a public domain code that is part of a system of software that is known as the Computer-Aided Management of Emergency Operations (CAMEO) that was developed to plan for and respond to chemical emergencies. It is also widely used throughout the DOE complex for safety analysis applications, which is the focus of this document. The United States Environmental Protection Agency (EPA), through its Chemical Emergency Preparedness and Prevention Office (CEPPO), and the National Oceanic and Atmospheric Administration Office of Response and Restoration (NOAA) jointly sponsor ALOHA. ALOHA can be downloaded free of charge from the EPA website (http://www.epa.gov/ceppo/cameo/aloha.htm). An accompanying user's manual can also be obtained at the website (NOAA, 1999a). An online help is also built into the code and a technical staff is available to address user questions (NOAA, 1999b).

The ALOHA code has evolved over the years to add capabilities, improve algorithms, and fix errors. Appendix C contains a reproduction of website information on the developmental history of the ALOHA code from the early 1980s to the present. (http://response.restoration.noaa.gov/cameo/alohafaq/history.html).

ALOHA runs either on Macintosh or in Microsoft Windows™ (version 95 or later) on IBM-compatible personal computers. ALOHA requires a least 1 megabyte (MB) of RAM and about 2.5 MB of hard disk space.

Information sources for the technical details of the ALOHA algorithms are from the ALOHA User's manual (NOAA, 1999a), the online help with ALOHA 5.2.3 (NOAA, 1999b), the APAC WG reports (Brereton, 1997; Lazaro, 1997), a NOAA report (Evans, 1993) and a draft NOAA theoretical description memorandum (for ALOHA 5.0) (Reynolds, 1992). Information from ALOHA websites is also used:

- http://www.epa.gov/ceppo/cameo/instruct.htm
- http://www.nwn.noaa.gov/sites/hazmat/cameo/aloha.html
- http://response.restoration.noaa.gov/cameo/aloha.html

Whenever possible, an attempt was made to verify any information that was in the draft NOAA theoretical description memorandum through use of the others sources of information.

2.2 Overview of ALOHA Models

Specifically, ALOHA performs calculations for source terms and downwind concentrations. Source term calculations determine the rate at which the chemical material is released to the atmosphere, release duration, and the physical form of the chemical upon release.[1] The term cloud is used in this document to refer to the volume that encompasses the chemical emission. In general, the released chemical may be a gas, a vapor, or an aerosol. The aerosol release may consist of either solid (e.g., fume, dust) or liquid (e.g., fog, mist, spray) particles that are suspended in a gas or vapor medium.[2] Liquid particles are also referred to as droplets.

The analyst specifies the chemical and then characterizes the initial boundary conditions of the chemical with respect to the environment through the source configuration input. The ALOHA code allows for the source to be defined in one of four ways (i.e., direct source, puddle source, tank source, or pipe source) in order to model various accident scenarios. The source configuration input is used to either specify the chemical source term or to provide ALOHA with the necessary information and data to calculate transient chemical release rates and physical state of the chemical upon release. ALOHA calculates time-dependent release rates for up to 150 time steps (NOAA, 1999a). Each time step typically lasts long enough for one percent of the potential chemical mass to be released to the atmosphere (NOAA, 1999a). ALOHA then averages the release rates from the individual time steps over one to five averaging periods, each lasting at least one minute (NOAA, 1999a). The five averaging periods are selected to most accurately portray the peak emissions. The five average release rates are inputs to the ALOHA algorithms for atmospheric transport and dispersion (NOAA, 1999a). ALOHA tracks the evolution of the mean concentration field of the five separate chemical clouds and calculates the concentration at a given time and location through superimposition. ALOHA limits releases to one hour.

Evolution of the mean concentration field of the chemical cloud is calculated through algorithms that model turbulent flow phenomena of the atmosphere. The prevailing wind flows and

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[1] More sophisticated source term algorithms that are found in other computer codes will also model the energetic effects of the release (e.g., as would occur with a fire or explosion) to include the impact of the initial momentum and buoyancy. ALOHA ignores these effects that can lead to initial puff or plume rise, which is sometimes modeled through an effective, elevated release height. The ALOHA approach of ignoring initial puff or plume rise is conservative in accident analysis applications since the ground-level concentration will be less with an elevated release with respect to a ground-level release when plume depletion from deposition effects are ignored, as is done in ALOHA.

[2] The ALOHA code user’s manual cautions that the ALOHA code does not model particulate transport phenomena (e.g., gravitational settling). Generally, particulate transport phenomena can be ignored with little error, but it is up to the analyst to make a determination of whether a passive atmospheric transport or dense-gas transport model is most appropriate. ALOHA has both models, and information in this document will provide guidance on their use. In the case of low concentrations of very fine airborne particles, it is reasonable to neglect transport phenomena peculiar to particulate and to assume that the particles remain suspended and act as a passive scalar contaminant that follows the flow field (Hanna, 2002). Under high concentrations of particles, the density of the cloud may be high enough that dense gas transport phenomena may be important.

associated atmospheric turbulence serve to transport, disperse[3], and dilute the chemical cloud that initially forms at the source. For an instantaneous release or release of short duration, the chemical cloud will travel downwind as a puff. In contrast, a plume will form for a sustained or continuous release.

The wind velocity is a vector term defined by a direction and magnitude (i.e., wind speed). The wind direction and wind speed determine where the puff or plume will go and how long it will take to reach a given downwind location. For sustained or continuous releases, the wind speed has the additional effect of stretching out the plume and establishing the initial dilution of the plume (i.e., determines the relative proportion of ambient air that initially mixes with the chemical source emission). Atmospheric turbulence causes the puff or plume to increasingly mix with ambient air and grow (disperse) in the lateral and vertical direction as it travels downwind. Longitudinal expansion also occurs for a puff. These dispersion effects further enhance the dilution of the puff or plume. The two sources of atmospheric turbulence are mechanical turbulence and buoyant turbulence. Mechanical turbulence is generated from shear forces that result when adjacent parcels of air move at different velocities (i.e., either at different speeds or directions)[4]. Fixed objects on the ground such as trees or buildings increase the ground roughness and enhance mechanical turbulence in proportion to their size. Buoyant turbulence arises from vertical convection and is greatly enhanced by the formation of thermal updrafts that are generated from solar heating of the ground.

The ALOHA code considers two classes of atmospheric transport and dispersion based upon the assumed interaction of the released cloud with the atmospheric wind flow.

- For airborne releases in which the initial chemical cloud density is less than or equal to that of the ambient air, ALOHA treats the released chemical as neutrally buoyant.[5] A neutrally buoyant chemical cloud that is released to the atmosphere does not alter the atmospheric wind flow, and therefore, the term passive is used to describe the phenomenological characteristics associated with its atmospheric transport and dispersion. As a passive

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[3] The term dispersion is sometimes used in the literature to describe the combined effects of advection (transport by the bulk motion of the wind flow) and turbulent diffusion (spreading) and other times, particularly in meteorological publications, to describe only the turbulent diffusion component. The latter, narrower sense is used in this document.

[4] Atmospheric flows experience a change in speed with height due to the friction of the earth's surface in slowing down the wind adjacent to it.

[5] In the strictest sense, neutrally buoyant conditions exist when the density difference between the released chemical cloud and ambient air is small. A positively buoyant cloud is produced when the cloud density is significantly less than that of the ambient air. The positive buoyancy induces puff or plume rise that results in an effective elevated release. The ALOHA code does not account for these positive buoyancy effects, but instead models the release as neutrally buoyant. This approach is conservative in accident analysis applications since the ground-level concentration will be less with an elevated release with respect to a ground-level release.

contaminant, the released chemical follows the bulk movements and behavior of the atmospheric wind flow.

- Conversely, if the density of the initial chemical cloud is greater than that of the ambient air, then the possibility exists for either neutrally buoyant or dense-gas type of atmospheric transport and dispersion.[6] In dense-gas atmospheric transport and dispersion, the dense-gas cloud resists the influences of the hydraulic pressure field associated with the atmospheric wind, and the cloud alters the atmospheric wind field in its vicinity. Dense-gas releases can potentially occur with gases that have a density greater than air due to either a high molecular weight or being sufficiently cooled. A chemical cloud with sufficient aerosol content can also result in the bulk cloud density being greater than that of the ambient air. Dense-gas releases undergo what has been described in the literature as "gravitational slumping". Gravitational slumping is characterized by significantly greater lateral (crosswind) spreading and reduced vertical spreading as compared to the spreading that occurs with a neutrally buoyant release.

Appendix A contains a more in-depth discussion of the neutrally buoyant model and the dense gas model that are used in ALOHA for atmospheric transport and dispersion calculations.

In addition to the source term and downwind concentration calculations, ALOHA allows for the specification of concentration limits for the purpose of consequence assessment (e.g., assessment of human health risks from contaminant plume exposure). ALOHA refers to these concentration limits as level-of-concern (LOC) concentrations. Safety analysis work uses the emergency response planning guidelines (ERPGs) and temporary emergency exposure limits (TEELs) for assessing human health effects for both facility workers and the general public (Craig, 2001). While ERPGs and TEELs are not explicitly a part of the ALOHA chemical database[7], ALOHA allows the user to input an ERPG or TEEL value as the LOC concentration. The LOC value is superimposed on the ALOHA generated plot of downwind concentration as a function of time to facilitate comparison. In addition, ALOHA will generate a footprint that shows the area (in terms of longitudinal and lateral boundaries) where the ground-level concentration reached or exceeded the LOC during puff or plume passage (the footprint is most useful for emergency response applications) (Figure 2-1).

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[6] ALOHA uses the terminology heavy gas in place of dense gas.

[7] The ALOHA chemical database incorporates two sets of concentration limits that are used in the chemical industry to address worker safety issues: (1) immediately dangerous to life or health (IDLH) and (2) threshold limit value – time weighted average (TLV-TWA).

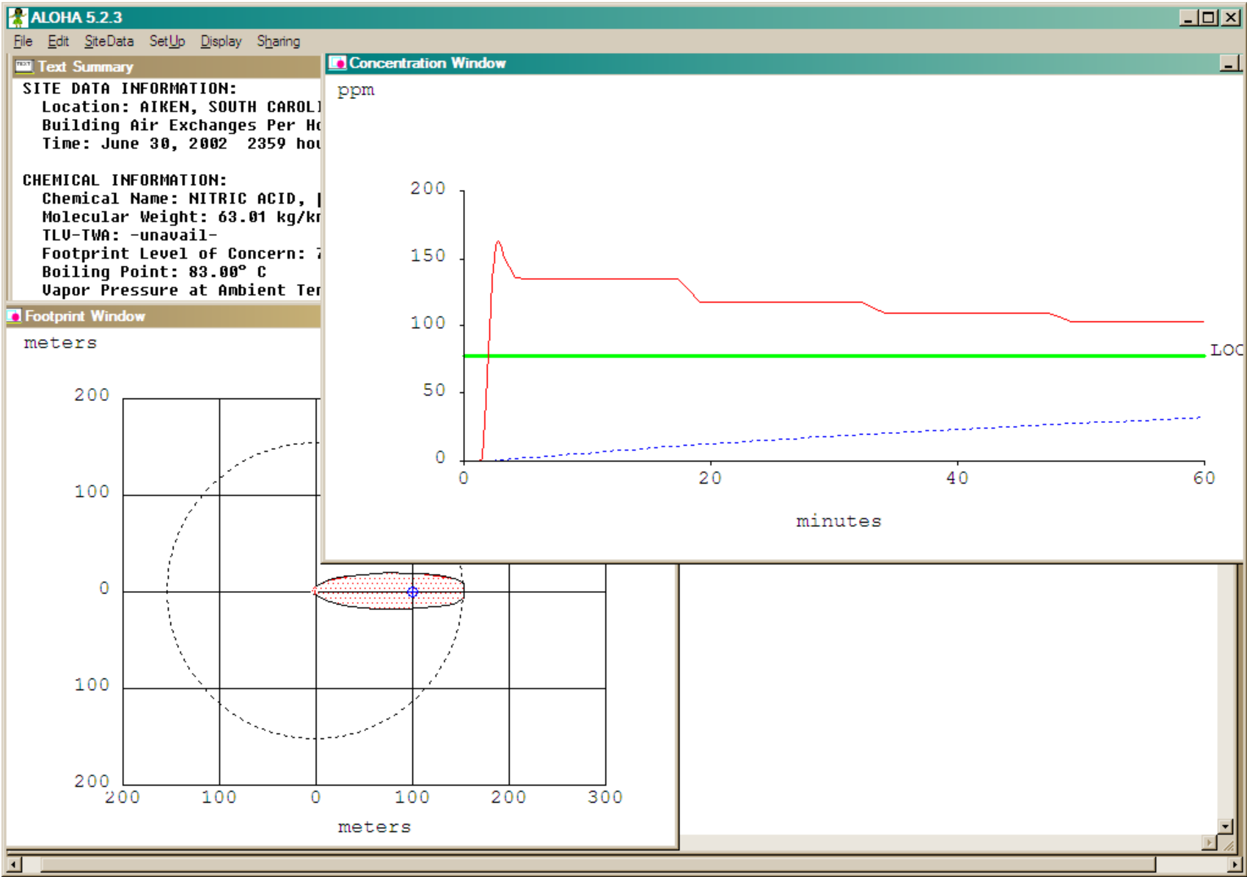

Figure 2-1. ALOHA Graphical Output.

2.3 ALOHA Software Quality Assurance

The validation and verification (V&V) efforts for ALOHA are not formally documented and do not appear to be part of a systematic quality assurance (SQA) plan (DNFSB, 2000). Some SQA information can be found in a document that is posted on the NOAA website as summarized below (NOAA, 1998). Benchmark comparisons have been made with the results from the ARCHIE (FEMA, 1989) and CHEMS-PLUS (Little, 1998) computer models. Results from the benchmark comparisons are not reported (NOAA, 1998). Comparisons with field data were also made with the following results reported (NOAA, 1998).

- Source term prediction for non-boiling pool evaporation – All ALOHA predictions were within 42% of measured evaporation rates.
- Source term prediction for liquefied propane – About 83% of ALOHA predictions were within a factor of two of measured vaporization rates.
- Atmospheric transport and dispersion predictions with Gaussian model – ALOHA predictions of mean downwind concentrations were on average 142% of the measured field

data. ALOHA tended to underestimate concentrations at distances of 200 meters or more and overestimate concentrations closer in.

- Atmospheric transport and dispersion predictions with dense-gas model – ALOHA predictions were not compared directly with field measurements, but compared with results from the DEGADIS model that was calibrated to 12 trials from field experiments (Spicer, 1989). ALOHA predictions of mean downwind concentrations were on average 107% of DEGADIS predictions, and about 70% of DEGADIS predictions were within a factor of two of measured field concentrations.

Atmospheric transport and dispersion predictions with dense-gas model for hydrogen flouride (HF) releases – ALOHA predictions were not compared directly with field measurements, but compared with results from the DEGADIS model that was calibrated to 12 trials from field experiments (Spicer, 1989). ALOHA predictions of mean downwind concentrations were on average 48% of the measured field data.

3.0 APPLICABLE REGIMES

The objective of this section is to present a discussion of ALOHA applicability from two perspectives: (1) in terms of its overall function as a key step in accident analysis; and (2) noting the phenomenological regimes in which it provides an approximate model of dispersion in the environment and the resulting toxicological exposure to downwind individuals (receptors).

3.1 Overall Application in Safety Analysis

The ALOHA code in the toolbox under the area of applicability of chemical release and dispersion and consequence. A code of this type of is used primarily to calculate the release rate to the atmosphere of a chemical involved in an accident scenario and the resulting instantaneous or time-averaged concentration of a chemical downwind from the accident. Because the DOE does not have an evaluation guideline for chemicals, the chemical concentration calculated is not used to distinguish safety-class designation for systems, structures, and components. Therefore, the quality of the numbers does not affect this portion of the safety process.

Occasionally, chemical concentrations are used to help set limits on chemical inventory, and this may present more of a safety implication. When these code calculations are used to help set inventory limits, they have a direct effect on values used in technical safety requirements, and the quality of the calculation may be very important. Again, it is important to note that a hand calculation can be used to verify this value. In this context of setting limits on chemical inventory, analysts have generally applied the emergency response planning guidelines (ERPGs) and temporary emergency exposure limits (TEELs) for the purpose of assessing human health effects for both facility workers and the general public (Craig, 2001). Since the DOE has not provided definitive evaluation guidelines for chemical exposures, the specific use of ERPGs and TEELs in accident analysis remains largely an open issue. It is recommended that guidance from subject-matter experts be followed (Craig, 2001). In some cases, surrogate values for inventory limits (such as EPA or OSHA limits) can also be used.

Phenomenological Regimes of Applicability

The atmospheric transport and dispersion algorithms of ALOHA are based on the Gaussian models for puffs and plumes and on dense-gas models. These models are best suited for specific types of conditions. The chief phenomenological regimes for applying ALOHA include:

- Temporal regime – The use of these models is best suited for "short" duration plumes, ranging from approximately several minutes to several hours (ALOHA limits the duration to one hour).

- Spatial regime - The atmospheric transport and dispersion models have high uncertainty close to the source, especially where the influence of structures or other obstacles is still significant. Dispersion influenced by several, collocated facilities, within several hundred meters of each other should be modeled with care. Similarly, ALOHA imposes a downwind distance limit of ten kilometers (six miles). The rationale behind the distance limit of ten kilometers and the one-hour time limit that is noted above is that meteorological conditions are likely to vary with location and change after significant passage of time. Long-range projections of toxicological exposures are better calculated with mesoscale, regional models that are able to account for multiple weather observations.

- Terrain variability – The atmospheric transport and dispersion models of ALOHA are inherently flat-earth models, and perform best over regions of transport where there is minimal variation in terrain.

- Extreme weather – The atmospheric transport and dispersion models of ALOHA do not apply to extreme weather conditions such as tornadoes. Appendix B summarizes an approach that has been used at Savannah River Site for tornadoes.

4.0 INPUTS AND RECOMMENDATIONS

4.1 Overview of ALOHA Input Menus

Users of ALOHA enter input data mainly through two menus that are labeled "Site Data" and "Set up" on the menu bar (Figure 4-1). Preliminary information about the location of the accidental release and date and time are entered through a series of dialog boxes that are accessed through the Site Data menu. The chemical that is released and the initial and boundary conditions associated the postulated accident scenario are input through a series of dialog boxes that are accessed through the Set up menu. In addition, an ERPG or TEEL value can be entered as the LOC value under the menu labeled "Display" ("Options" submenu).

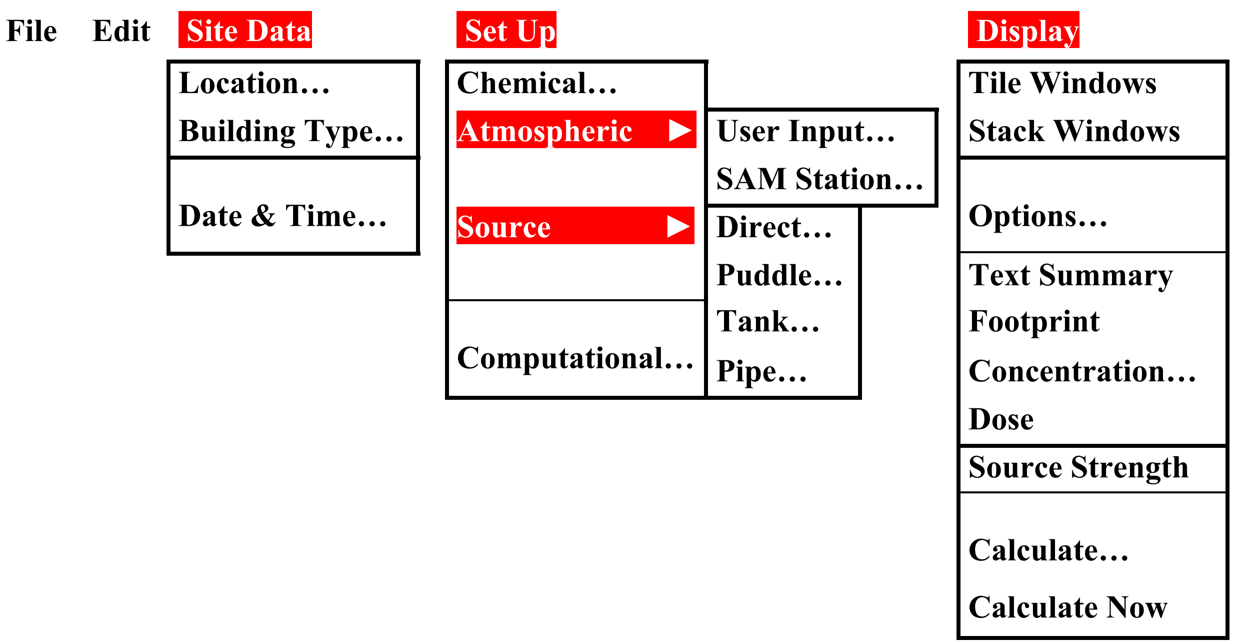

Figure 4-1. ALOHA Menu Bar.

For each numerical input, ALOHA typically allows for a variety of units (both metric and British) to be used. The user must therefore identify the particular units to be used among those offered by ALOHA and input the numerical value on the basis of the units that have chosen for the given input parameter. Frequently, an ALOHA dialog box presents one or more pre-defined options that the user may select through the use of selection bubbles, but generally the user is not limited to these options as a space for numerical values to be input as an alternative is usually available (Figure 4-2).

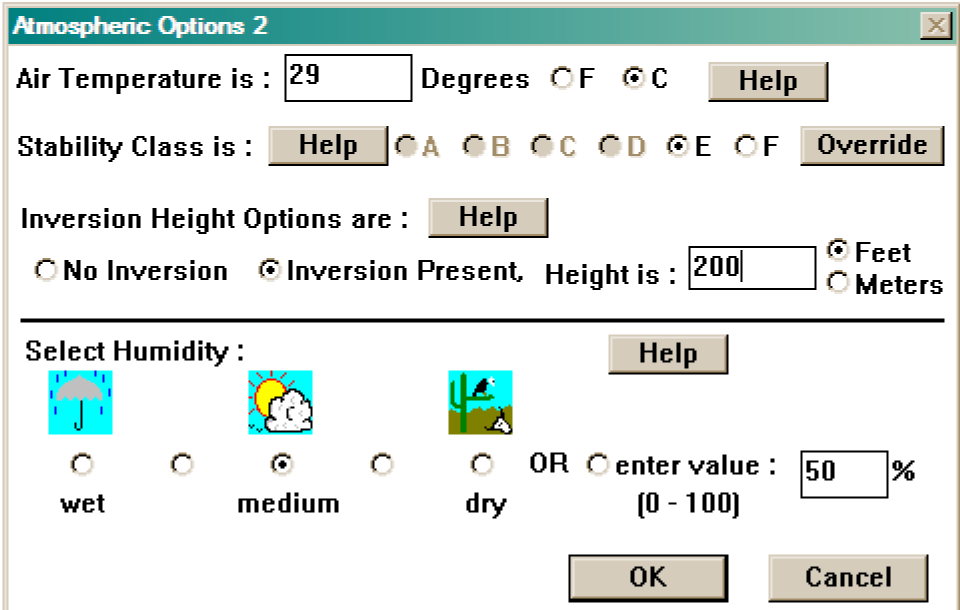

Figure 4-2. Sample ALOHA Dialog Box for Data Entry.

4.2 Input Recommendations for Site Data Parameters

The following submenus are included under the Site Data menu:

- Location
- Building Type
- Date and Time

4.2.1 LOCATION

More than 500 U.S. cities as well as some Canadian cites are part of the ALOHA library. The library includes the elevation, longitude, and latitude of each city. The longitude and latitude, along with the time and date inputs that are discussed later, are used to estimate the incoming solar radiation (Reynolds, 1992). The amount of incoming solar radiation on a puddle influences the evaporation rate. ALOHA uses the elevation input to determine ambient air pressure (Reynolds, 1992).

Recommendation: Choose the city in closest proximity to the location of interest or add a new city to the library by entering its name along with the elevation, longitude, and latitude of the city.

4.2.2 BUILDING TYPE

Building parameters related to infiltration are entered through the dialog box under the Building Type submenu. Choices for the building type are (i) enclosed office building, (ii) single storied building, or (iii) double storied building. The user selects one the above three choices or alternatively enters the number of air changes per hour (allowable range is 0.01 to 60 exchanges per hour) (NOAA, 1999b). The user also identifies the building surroundings as either sheltered (with trees, bushes, etc.) or unsheltered.

Recommendation: ALOHA uses the information entered here to determine indoor infiltration and to estimate indoor concentration and chemical dose at a location. ALOHA assumes that all doors and windows are closed. DSA analysis conservatively takes no credit for sheltering or evacuation. As a result, safety analysts do generally not use the indoor concentration and chemical dose calculated by ALOHA.

4.2.3 DATE AND TIME

The user is provided with the option to use either the internal clock or set a constant time and date. Time is based on a 24-hour clock. ALOHA uses this input, along with the location data, to determine the incoming solar radiation based upon the position of the sun.

Recommendation: Set a constant time that is consistent with the input specification for the atmospheric stability class (discussed in a later section). For example, stable atmospheric conditions occur at night or early morning. Unstable atmospheric conditions occur during the day. Neutral atmospheric conditions can occur either at day or night. For analysis of a daytime release, the evaporation rate increases with increasing solar influx. A conservative approach for unstable and neutral atmospheric conditions is to set the date to a mid-summer day (e.g., June 30th) and the time to around noon (e.g., 12:00). Any year may be specified since the results can be expected to be insensitive to the year input (ALOHA, however, will prompt the user to check his entry if the year is more than 10 years away from the current year).

4.3 Input Recommendations for Set Up Parameters (Scenario Definition)

The following submenus are included under the Set Up menu:

- Chemical Information
- Atmospheric Options
- Source
- Computational Preferences

4.3.1 CHEMICAL INFORMATION

Over 1000 chemicals are part of the chemical library.

Recommendation: Choose chemical of concern from chemical library list or enter new chemical into library. An ALOHA dialog box will prompt the user to enter the following information for the new chemical.

- Chemical name
- Molecular weight
- Boiling point
- Critical pressure
- Critical temperature
- Default level of concern
- Density (gas)
- Density (liquid)
- Diffusivity (molecular)
- Freezing point (normal)
- Heat capacity (gas, constant pressure)
- Heat capacity (liquid, constant pressure)
- IDLH
- TLV-TWA
- Vapor pressure

Information on what properties are required to support each source configuration option and atmospheric transport and dispersion type is given in Table 4-1 (NOAA, 1999a).

Table 4-1 Use of Chemical Property Data

Property	Direct Source		Puddle Source		Tank Source		Pipe Source	
	Gaussian	Heavy Gas	Gaussian	Heavy Gas	Gaussian	Heavy Gas	Gaussian	Heavy Gas
Chemical Name	●	●	●	●	●	●	●	●
Molecular Weight	●	●	●	●	●	●	●	●
Boiling Point	●[1]	●	●	●	●	●	●	●
Critical Pressure	●[1]	●[2]	●	●	●	●	●	●
Critical Temperature	●[1]	●[2]	●	●	●	●	●	●
Gas Density		●		●		●		●
Freezing Point			●	●	●	●		
Gas Heat Capacity		●	●	●	●	●	●	●
Liquid Heat Capacity			●	●	●	●		
Vapor Pressure		●[2]						

1 Required only if direct source term is expressed in volume or volume rate units. That is, these properties are not required if source term is expressed in mass or mass rate units.

2 Either the vapor pressure is required or both the critical pressure and critical temperature is required.

4.3.2 ATMOSPHERIC OPTIONS

ALOHA allows meteorological conditions to be entered from a portable monitoring station. For accident analysis purposes, however, the user enters the meteorological data manually. Note that ALOHA does not handle extreme weather conditions such as tornadoes Appendix B summarizes an approach that has been used at Savannah River Site for tornadoes.

ALOHA requires input for the following meteorological parameters.

- Wind speed

- Wind direction
- Measurement height of wind speed
- Ground roughness
- Cloud cover
- Air temperature
- Stability class
- Inversion height
- Humidity

In calculating puff or plume concentrations, both "unfavorable" and "typical" dispersion conditions are of special interest in accident analyses. For accident analysis consideration of the offsite receptor, unfavorable meteorology is ideally based on site data. In defining unfavorable meteorological conditions for chemical releases, it seems reasonable to follow the practices that are used for radiological consequence analysis. Unfavorable meteorology refers to the meteorology that coupled with the source term would lead to doses (or concentration exposures for chemicals) that are exceeded less than five percent of the time. The method should be conservative or consistent to the discussion in the NRC Regulatory Guide 1.145 (Position 3) (NRC, 1983) as summarized in Appendix A to DOE-STD-3009-94, CN2 (DOE, 2002a). The 95^{th} percentile of the distribution of doses (or concentration exposures for chemicals) to the offsite receptor, accounting for variation in distance to the site boundary as a function of direction, is the comparison basis for assessment against the evaluation guidelines. Typical meteorological conditions are sometimes used for consequence analysis of the onsite worker. The median or the 50^{th} percentile of the distribution is usually the basis for typical meteorological conditions.

Meteorological variables such as wind speed and solar radiation affect both the evaporation rate and the amount of dilution of the puff or plume during atmospheric transport. Generally, these variables affect the evaporation rate and atmospheric dilution in opposite ways with regard to the effect produced on downwind concentrations. For example, higher wind speeds increase the evaporation rates, but also support greater dilution of the plume. Similarly, higher solar radiative influx and warmer temperatures also increase the evaporation rates, but typically support atmospheric conditions that are less stable and more dispersive. Meteorologists at Savannah River Site (SRS) studied these effects and concluded that the dominant influence of the meteorological variables generally occurs with atmospheric dispersion and dilution (Hunter, 1993). Higher downwind concentrations are associated with stable atmospheric conditions and low wind speeds (Hunter, 1993).

The size of the data set used in the meteorological assessments should be sufficiently large that it is representative of long-term meteorological trends at most sites. Meteorological data, qualified and meeting requirements of Regulatory Guide 1.23 (NRC 1972), available at most DOE sites should be applied that is representative of long-term trends. A five-year data set is desirable, but a one-year data set can be applied under the right circumstances.[8]

In lieu of site-specific meteorology, the accident analysis may use generally accepted, default stability and wind speed combinations. For example, F stability class and 1.5 m/s wind speed is recommended by the EPA for analysis of ground-level releases of neutrally buoyant plumes (EPA, 1996). See Appendix A for a fuller discussion on the role of wind speed and atmospheric stability class on downwind puff or plume concentrations, especially as these parameters relate to the Gaussian transport and dispersion models for neutrally buoyant releases. For elevated releases, the lofted plume must travel further downwind with stable atmospheric conditions before reaching the ground and exposing receptors to the hazardous contaminant. Therefore, neutral or even unstable stability conditions may produce the most unfavorable meteorological conditions for receptors close to the elevated release.

It should be noted that in the long run, site data is normally preferable over the default conditions for accident analysis. Meteorologists evaluated SRS data and found the 95th percentile conditions varied with release height, and receptor distance (Hunter, 1993). For most facility distances to the offsite boundary, it was determined that 95th percentile conditions for neutrally buoyant plumes were E stability and the following wind speeds.[9]

- 1.7 m/s wind speed (release height 0 m – 10 m)
- 2.1 m/s wind speed (20-m release height), and
- 3.0 m/s wind speed (60-m release height).

For mitigated hazard analysis, DOE has not established prescriptive guidance for evaluating the mitigated benefit of safety structures, systems, and components (SSCs). Both median statistical basis (i.e., 50th percentile) and 95th percentile bases have been applied to determine onsite receptor doses.

Finally, note that the specification of the atmospheric stability class in ALOHA should be consistent with inputs for location, date and time, wind speed, surface roughness length, and cloud cover. Algorithms are used within ALOHA to inform the user of which atmospheric stability classes are appropriate based upon data that the user has entered for these other parameters.

Guidance for each meteorological parameter required by ALOHA follows.

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[8] In Draft Regulatory Guide DG-111, this subject is discussed as follows: "The NRC staff considers five years of hourly observations to be representative of long-term trends at most sites. With sufficient justification of its representativeness, the minimum meteorological data set is one complete year (including all four seasons) of hourly observations." (NRC, 2001)

[9] The cited wind speeds reflect the value at the release height (at 10 m for the 0 m – 10 m release height range).

Wind Speed

ALOHA accepts 10-m reference elevation wind speeds in the range of 1 m/s to 60 m/s (NOAA, 1999b). ALOHA can accommodate wind speed values that are representative of other heights since inputs are required for both the wind speed and the corresponding height for this wind speed. The height input parameter for the wind speed is discussed separately in a later section of this document.

Recommendation: As discussed above, statistical analysis of site-specific, wind speed measurements is the preferred approach for specifying wind speed. The determination of the 50th and 95th percentile meteorological conditions will require the simultaneous consideration of both atmospheric stability class and wind speed (ambient temperature may also be considered for scenarios that involve pool evaporation).

In general, higher downwind concentrations (i.e., unfavorable meteorological conditions) are associated with lower wind speeds. In lieu of site-specific meteorological data, the following default wind speeds may be considered for each atmospheric stability class (Lazaro, 1997). More discussion of the interplay between wind speed and atmospheric stability in establishing typical and unfavorable meteorological conditions is presented later in the context of the input for atmospheric stability class. Also, performing a parametric study among the various combinations of wind speed and atmospheric stability classes can provide useful insights about the role of wind speed and atmospheric stability class in determining unfavorable meteorological conditions.

	Atmospheric Stability Class					
	A	B	C	D	E	F
Default Wind Speed [m/s]	2.0	*	*	4.5	1.5	1.5

* Lazaro (1997) does not specify default wind speeds for B and C stability classes. The 2.0 m/s default wind speed value that is specified for A stability class would seem to be a reasonably conservative choice based on information presented later in this section, as well as in Appendix A, for atmospheric stability class and wind speed.

Wind Direction

The wind direction is specified as the direction from which the wind is blowing. You can enter this information in either units of degrees true, or in one- to three-letter directional terms. For example, you can indicate that the wind is blowing from the north-northeast by entering either NNE or 22.5 degrees.

Wind directions expressed in degrees and letter terms correspond as follows:

- N = 0 degrees or 360 degrees
- NNE = 22.5 degrees
- NE = 45 degrees

- ENE = 67.5 degrees
- E = 90 degrees
- ESE = 112.5
- SE = 135 degrees
- SSE = 157.5 degrees
- S = 180 degrees
- SSW = 202.5 degrees
- SW = 225 degrees
- WSW = 247.5 degrees
- W = 270 degrees
- WNW = 292.5 degrees
- NW = 315 degrees
- NNW = 337.5 degrees

Recommendation: For accident analysis calculations, any direction may be input. The calculated concentrations for a given downwind distance that are calculated by ALOHA are insensitive to direction input.

Measurement Height for Wind Speed

ALOHA accounts for the variation of wind speed with distance from the earth's surface as caused by friction.

Recommendation: The input for this parameter must be consistent with the value that is input for the wind speed (that was discussed in a previous section above). If the value for wind speed input into ALOHA is based on site measurements at a known height, then that height should be input. Generally, portable weather monitoring stations are mounted on stand that is approximately 3 meters high. Typically, the NWS measures and reports wind speeds at 10 meters.

Ground Roughness

ALOHA accepts input of surface roughness length (z_o) between 0.001 centimeters and 200 centimeters. (NOAA, 1999b). How ALOHA uses this input depends upon whether ALOHA is performing a heavy-gas or Gaussian dispersion calculation as discussed below (NOAA, 1999b).

For a heavy-gas dispersion calculation, ALOHA limits z_o to 10 centimeters. ALOHA will set z_o to the value entered by the user when the value is 10 centimeters or less. ALOHA uses a maximum z_o value of 10 centimeters whenever the user enters a value that is greater than 10 centimeters.

For a Gaussian dispersion calculation, ALOHA will either use a z_o value of 3 centimeters or 100 centimeters. The 3-cm value corresponds to terrain that is characterized as "open country". In open country, the roughness elements are small and widely spaced (e.g., open fields, parking lots). The 100-cm value corresponds to terrain that is characterized as "urban or forest" and that would be characteristic of residential housing developments, industrial areas or forests. ALOHA will set z_o to the 3-cm value whenever the user enters a value that is 20 centimeters or less. ALOHA uses a z_o value of 100 centimeters whenever the user enters a value that is greater than 20 centimeters. Recall published literature suggests that the dependence of σ_z on z_o can be approximated by a factor proportional to $(z_o)^{0.2}$ and that downwind concentrations are inversely proportional to σ_z in the Gaussian dispersion equation. As a result, open country (z_o = 3 cm) Gaussian dispersion calculations can be expected to produce downwind concentrations that are roughly double those calculated for urban or forest dispersion (z_o = 100 cm) since the result of $(100/3)^{0.2}$ approximately equals 2.[10]

The different approaches for heavy-gas dispersion and Gaussian dispersion is consistent with the observation that surface roughness has less influence on dense-gas releases in comparison with neutrally buoyant releases (Lazaro, 1997).

Recommendation: It is conservative to always choose open country dispersion (or equivalently specify a z_o value of 3 cm) instead of urban or forest dispersion (z_o = 100 cm). It is recommended, however, that the analyst uses judgment based on site observation and published guidance to take credit for surface roughness effects in increasing puff and plume dispersion where appropriate.

The ALOHA online help recommends using the dominant characteristic of the terrain that surrounds the postulated release and receptor distances of interest (NOAA, 1999b). Following this guidance, urban or forest terrain would be selected whenever more than 50% of the surrounding terrain is urban or forest.

Alternatively, the user may input a z_o value. Various tables of z_o as a function of terrain attributes are found in the literature (Lazaro, 1997; Hanna, 2002). In addition, the ALOHA online help (NOAA, 1999b) provides the following guidance from Brutsaert (1982).

Surface description	z_o (cm)
Mud flats, ice	0.001
Smooth tarmac (airport runway)	0.002
Large water surfaces (average)	0.01-0.06

[10] ALOHA uses the same set of σ_y curves for both open country and urban applications (Reynolds, 1992).

Grass (lawn to 1 cm high)	0.1
Grass (airport)	0.45
Grass (prairie)	0.64
Grass (artificial, 7.5 cm high)	1.0
Grass (thick to 10 cm high)	2.3
Grass (thin to 50 cm)	5.0
Wheat stubble plain (18 cm)	2.44
Grass (with bushes, some trees)	4
1-2 m high vegetation	20
Trees (10-15m high)	40-70
Savannah scrub (trees, grass, sand)	40
Large city (Tokyo)	165

<u>Cloud Cover</u>

This input parameter represents the proportion of the sky that is covered by clouds. It is expressed in tenths following the convention that is used by U.S. meteorologists. For example, 5 tenths corresponds to a sky that is half-covered by clouds. The allowable input range is from 0 (completely clear sky) to 10 (completely cloudy sky). ALOHA uses this input to estimate the amount of incoming solar radiation that is incident upon the puddle formed by a liquid spill. Decreasing cloud cover allows for more heating of the puddle by the sun and a higher evaporation rate. The calculation uses this input for the release scenarios that involve a puddle forming on the ground (e.g., specified explicitly by user through puddle source or determined by ALOHA with a user-specified tank source). Although not used for scenarios that do not involve a puddle (e.g., direct source, pipe source), a value for the fractional cloud cover is still required by ALOHA.

Recommendation: The specification of fractional cloud cover should be consistent with the atmospheric stability class input. Stable and unstable atmospheric conditions are supported by low cloud cover conditions. For daytime releases, some minimum amount of cloud cover may be necessary to support neutral (class D) atmospheric conditions.

For releases that are postulated to occur at night (e.g., under stable meteorological condition), the downwind concentrations calculated by ALOHA are insensitive to the fractional cloud cover since the incoming solar radiation is not a factor in determining the evaporation rate.

For releases that involve puddles and that are postulated to occur during the day, the evaporation rate is sensitive to the incoming solar radiation. A recommended conservative approach is based upon algorithms that are used in ALOHA to identify appropriate choices for atmospheric stability class based on the inputs for location, date and time, wind speed, surface roughness length, and cloud cover. Using the data entered for these other input parameters, ALOHA dims the stability class designations that it determines to be incompatible (and fills the associated selection bubble gray as shown in Figure 4-2) and leaves the other stability classifications available for selection (clear selection bubble).[11] A trial-and-error approach for specifying a conservative fractional cloud cover use with daytime puddle scenarios is outlined below.

- Following guidance that is in this document, determine the combination of atmospheric stability class and wind speed that is appropriate for the accident scenario to be analyzed and type of meteorological conditions (e.g., unfavorable, typical) to be assumed for the analysis.

- Completely enter data under the Site Data menu, which will include the inputs for location and date and time.

- Under the Set Up menu, start entering data under the Atmospheric Options submenu in the order that ALOHA prompts the user through the dialog boxes: wind speed; wind direction; measurement height for wind speed; and then ground roughness length.

- Enter 0 (tenths) for fractional cloud cover. Observe the section of dialog box pertaining to atmospheric stability class to see if the atmospheric stability class of interest for the scenario is identified by ALOHA as compatible with the other inputs. If so, continue with the data entry thus using 0 tenths as the fractional cloud cover for the calculation. If not, increase the fractional cloud cover by 1 (tenth) until the atmospheric stability class of interest for the scenario is identified by ALOHA as compatible.[12]

Air Temperature

The allowable input range for air temperature is -100 degrees F to 150 degrees F (-73 degrees C to 65 degrees C) (NOAA, 1999b). Air temperature is an input to the puddle heat-transfer algorithm that is used to determine the puddle temperature, from which the vapor pressure of the liquid chemical and the evaporation rate are determined for non-boiling liquids.

Recommendation: As discussed above, statistical analysis of site-specific, meteorological measurements is the preferred approach for specifying meteorological conditions. For air temperature, a reasonably bounding high temperature is recommended based on analysis of the site data. For example, Lazaro suggests the 95th percentile of a five-year record of daily high temperatures for the warmest month of the year (Lazaro, 1997).

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[11] An override button allows the user to select any of the atmospheric stability classes that ALOHA has determined to be incompatible.

[12] If the atmospheric stability class of interest does not show up as compatible for any input value (0 to 10) for fractional cloud cover, check other input entries for correctness. The correctness check should include the date and time entries (note that if the user neglects to enter the date and time, ALOHA defaults to information supplied by the internal computer clock).

Stability Class

ALOHA uses data entered for date and time, wind speed, and cloud cover to identify stability classes that are compatible with the entered data and to automatically select a stability. ALOHA uses the table below for determining compatible stability classes (Turner, 1970; NOAA, 1999b).

Surface Wind	Day			Night	
Wind Speed	Incoming Solar Radiation			Cloud Cover	
[m/s]	Strong	Moderate	Slight	> 0.5	< 0.5
< 2	A	A-B	B	E	F
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
> 6	D	D	D	D	D

Notes for information above:

- Stability is D for completely overcast conditions during day or night.
- "Night" is the time period from 1 hour before sunset until 1 hour after sunrise.
- "Strong" solar radiation corresponds to clear skies with the sun high in the sky (solar angle greater than 60 degrees).
- "Slight" solar radiation corresponds to clear skies with the sun low in the sky (solar angle between 15 and 35 degrees).

Recommendation: As mentioned several times in this document, statistical analysis of site-specific, meteorological measurements is the preferred approach for specifying meteorological conditions. The determination of the 50^{th} and 95^{th} percentile meteorological conditions will require the simultaneous consideration of both atmospheric stability class and wind speed (ambient temperature may also be considered for scenarios that involve pool evaporation). In lieu of site-specific meteorological data, the following guidance is provided.

i) For ground-level (and nearly ground-level) releases that are neutrally buoyant, stable atmospheric conditions and low wind speeds represent generally accepted, unfavorable meteorological conditions (i.e., F stability class and 1.5-m/s wind speed) (Hanna, 1996a; Lazaro, 1997). Stable atmospheric conditions and low wind speeds are also expected to produce unfavorable meteorological conditions for dense gas releases at ground level that are continuous (Hunter, 1993; Hanna, 1996a; Lazaro, 1997).

ii) For short-duration releases (i.e., puffs) of dense gases, unfavorable meteorological conditions may occur with neutral stability conditions and moderate wind speeds (Hanna, 1996a; Lazaro, 1997). With dense-gas puffs, it is recommended that a parametric study be performed among the various combinations of wind speed and atmospheric stability classes to determine unfavorable meteorological conditions for the receptor locations of interest.

iii) For elevated releases of neutrally buoyant gases, the atmospheric stability class associated with unfavorable meteorological conditions will be dependent upon the distance of the receptor from the source. At very close distances, the ground level concentration may be zero for stable conditions as the puff or plume simply passes overhead. Unstable atmospheric stability will result in the highest ground-level concentrations at close distances as high levels of turbulence will promote rapid dispersion of the puff or plume to the ground from its elevated release position. At receptor locations further downwind, neutral atmospheric buoyant conditions produce the highest ground-level concentrations with the Gaussian plume model. Even further downwind, the highest ground-level concentrations occur with stable atmospheric conditions as the puff or plume has traveled far enough downwind for the puff or plume to disperse enough to reach ground level. With elevated releases of neutrally buoyant gases, it is recommended that a parametric study be performed among the various combinations of wind speed and atmospheric stability classes to determine unfavorable meteorological conditions for the receptor locations of interest.

As mentioned above, accident analysis calculations under typical meteorological conditions may sometimes be performed. Atmospheric stability class D is the most common stability class for many DOE sites. This is due to the large number of combinations that can result in stability class D. For example, high-wind conditions and/or cloudy conditions during the day or at night are normally associated with stability class D. A wind speed of 4.5 m/s together with atmospheric stability class has been suggested to represent typical meteorological conditions (FEMA, 1989). This set of conditions is also consistent with a basis by chemical process industry for determining limits on chemical inventories, and is representative of most U.S. regions (CFR, 1992) and for radiological hazard categorization of DOE facilities (DOE, 1997).

<u>Inversion Height</u>

ALOHA prompts the user for an inversion height or to indicate that no inversion exists. ALOHA accept input values for the inversion height between 10 feet (about 3 meters) and 5,000 feet (about 1,524 meters) (NOAA, 1999b).

A dense-gas cloud generally remains close to the ground as it travels downwind. As a result, ALOHA assumes that dense-gas dispersion in unaffected by the presence of an inversion layer (NOAA, 1999b). While this input is still required, ALOHA does not use the input value in the dense-gas dispersion calculations.

The presence of an inversion does restrict the upward dispersion of neutrally buoyant gases that is calculated by ALOHA. Increased ground-level concentrations may result due to the presence of the inversion.

The inversion layer height input that is used by ALOHA is frequently referred to as the mixing layer height. The mixing layer height varies throughout the day and throughout the seasons.

During clear nights or early mornings when inversions are present, the mixed layer is relatively low, while during sunny days the mixing layer is much higher. The magnitude of these heights can be obtained from balloon soundings or from remote sensing techniques, such as acoustic or radar soundings. In the absence of such data, regional tables can be consulted.

Recommendation: Base mixing layer height on seasonal averages and day/night time of day. Apply archived site or laboratory meteorological data. If this is not available, use regional data as default input values, such as those of Holzworth (1972).[13] Since lower inversion heights can lead to higher downwind concentrations, it is appropriate for conservatism to specify an inversion height value that is reasonable, but skewed more towards the lower end of the observed or expected range.

<u>Humidity</u>

A number of chemicals are hygroscopic and react with moisture in the air. Transformations that result can have a pronounced impact on atmospheric transport and dispersion, but these effects are not modeled in ALOHA.

ALOHA takes relative humidity into account when it estimates the rate of evaporation from a puddle. Specifically, the relative humidity affects longwave radiation transfer between the atmosphere and the puddle (Reynolds, 1992). Relative humidity also plays a role in heavy gas dispersion computations. When the cloud is at a temperature that is different than that of the ambient air, less air is required to mix with the cloud to achieve thermal equilibrium when the relative humidity is high since water has a significantly higher heat capacity relative to dry air (Lazaro, 1997).

The relative humidity is expressed as a percentage and entered as a whole number that is between 0 and 100 (percent) inclusive.

Recommendation: Neither the ALOHA documentation nor the published literature in general supply much detail on the role of water vapor content on calculations of chemical evaporation and subsequent transport and dispersion. The CDCA WG recommends a value of 50% for the relative humidity (Lazaro, 1997). In absence of other guidance, the use of a medium value for relative humidity seems reasonable. The user also has the option of using a value more

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[13] The mean mixing heights for mornings in the continental United States range between approximately 200 m and 1200 m depending upon season and location (Holzworth, 1972). The mean mixing heights are higher for afternoons, ranging between 500 m and 4000 m (Holzworth, 1972).

representative of the site being analyzed. Another alternative is to perform a parametric study on the sensitivity of the results to relative humidity for the accident being analyzed. [14]

4.3.3 SOURCE

The ALOHA code allows for the source to be defined in one of four ways in order to model various accident scenarios. These are:

- Direct source
- Puddle source
- Tank source
- Pipe source.

Recall that for chemical accident analysis, the source term[15] defines the quantity released to the atmosphere for an instantaneous release or the release rate to the atmosphere for a continuous release. If the source term is already known through measurement or calculation, then the analyst uses the direct source option to enter a constant source term. Otherwise, the analyst characterizes the initial boundary conditions of the chemical with respect to the environment through the source configuration in order to provide ALOHA with the necessary information and data to calculate a time-dependent chemical release rate and physical state of the chemical upon release. The initial boundary conditions are defined through input specifications as delineated through the puddle, tank, or pipe source configurations.

Depending upon the source configuration specified, the analyst is prompted to supply a particular set of initial conditions such as temperature and storage pressure (if applicable), and the ALOHA code sets physical and thermodynamic properties based on these inputs and information in the ALOHA chemical database. The possible physical state of the chemical in its initial condition is identified in brackets below for each of the four source configurations. Brief overviews of the four source configurations are given first, followed by more detailed descriptions.

(1) Direct source {gas}: A point source is defined for this source configuration as either an instantaneous (duration of one minute or less) or a continuous release of gas into the atmosphere. For an instantaneous release, the total amount of gas that is released is

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[14] The primary author of this document did a limited parametric study on the role of relative humidity on the downwind concentration for evaporation from 10-m diameter puddles of hydrazine and chlorine. The study assumed meteorological conditions of F atmospheric stability and 1.5-m/s wind speed. The evaporation of hydrazine, which has relatively low volatility, produced a cloud that ALOHA modeled as neutrally buoyant. Chlorine, which is much more volatile and has a higher molecular weight, produced a cloud that ALOHA modeled as a heavy gas. In each case, the downwind concentration at 100 m that was calculated by ALOHA varied less than 2% as relative humidity varied from 0% to 100%. Slightly higher concentrations occurred with the higher values of relative humidity.

[15] ALOHA uses the label "source strength" in place of "source term".

specified. For a continuous release, the release rate and duration are specified (up to one hour). In either case, a ground level or elevated release is specified. Also, the analyst identifies the release as undergoing neutrally buoyant dispersion or dense-gas dispersion. The analyst makes this determination based on calculation of the Richardson number (Ri), as described later.[16]

(2) Puddle source {liquid}: This source configuration represents evaporating or boiling liquid from a pool or puddle of a spilled chemical. The analyst specifies the liquid quantity and the puddle surface area as well as liquid temperature, ground temperature, and ground type. The ALOHA code uses these inputs together with chemical properties from the ALOHA chemical database to calculate the time-dependent evaporation rate (non-boiling conditions) or vaporization rate (boiling conditions).

(3) Tank source {gas, liquid, or liquefied gas}: In this source configuration, the ALOHA code calculates the discharge rate of the gas, liquid, or two-phase flow from a hole in a tank. The analyst specifies the tank dimensions, quantity stored, storage temperature (and storage pressure if a gas), and hole characteristics (size, shape, and location). For gases, vapors and aerosols that remain suspended in air upon exiting the tank, the calculated time-dependent discharge rate defines the release rate to the atmosphere. For liquid that is released from a tank and falls to the ground, additional calculations, besides the discharge rate from the tank, are needed to define the release rate to the atmosphere that occurs through evaporation or boiling. The spilled liquid will pool on the ground. Transient puddle development is modeled by ALOHA. The time-dependent evaporation rate (non-boiling conditions) or vaporization rate (boiling conditions) is calculated by ALOHA using essentially the same algorithms as used in the puddle source configuration.

(4) Pipe source {gas}: This source configuration represents gas discharges from a long pipe either (i) connected to a very large reservoir or (ii) disconnected from a source. Gas temperature and pressure are specified along with pipe dimensions (length and diameter) and relative surface roughness (i.e., smooth or rough).

Guidance for each source term configuration follows.

<u>Direct Source</u>

The direct source algorithm is used when the emission rate of the gas is known or calculated from manual calculations or another computer code. The emission rate remains constant throughout the duration of the release (up to one hour). The direct source is also the only option for modeling elevated releases.

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[16] For source configurations other than direct, the user inputs sufficient data to allow ALOHA to calculate the Ri number and to make a determination to model the release as neutrally buoyant or dense gas.

With the direct source, the analyst must specify the release as undergoing neutrally buoyant dispersion or dense-gas dispersion. The analyst makes this determination based on calculating the Ri number at the source (Ri_o), which is a relative measure of the potential energy of the cloud with respect to the mechanical turbulent energy of the atmosphere. Dense-gas behavior can potentially occur for gases with densities greater than air or with a chemical cloud with sufficient aerosol content such that the bulk cloud density is greater than that of the ambient air. Dense-gas behavior is more likely to occur with higher release rates and lower wind speeds. It is recommended that the analyst use the methodology used internally by the ALOHA code for other source configurations as a guide.

For source algorithms other than direct, the airborne release quantity or rate is calculated by the ALOHA code and used internally by ALOHA to determine Ri_o. The ALOHA code uses the following definitions of Ri_o for instantaneous and continuous releases, respectively.

For an instantaneous release (Reynolds, 1992):

$$Ri_o = \frac{g \times (\rho_o - \rho_a) \times Q_i}{\rho_a \times A_o \times u_*^2} \qquad (4\text{-}1)$$

Where, $\rho_a \equiv$ Ambient air density

$\rho_o \equiv$ Released chemical density at source

$Q_i \equiv$ Instantaneous volumetric release

$A_o \equiv$ Ground area of the source

$u_* \equiv$ Friction velocity

For a continuous release (Reynolds, 1992):

$$Ri_o = \frac{g \times (\rho_o - \rho_a) \times Q_c}{\rho_a \times D_o \times u_{10} \times u_*^2} \qquad (4\text{-}2)$$

Where, $Q_c \equiv$ Continuous volumetric release rate

$D_o \equiv$ Scale dimension of the source

$U_{10} \equiv$ Mean wind speed at a height of 10m

The friction velocity is equal to about 5% to 10% of the mean wind speed at the height of 10 m (Hanna, 1996a). The ALOHA code basis is 6.25% ($u_* = u_{10}/16$) (Reynolds, 1992). For a ground level release, the length scale parameter D_o represents the initial width or diameter of the cloud or plume before mixing with and transport by ambient air.[17] For a release out of a stack, D_o would represent the diameter of the stack (neglecting any boundary layer effects that would reduce the effective diameter of the jet or plume leaving the stack). For releases from evaporative or boiling pools, D_o is set equal to the pool diameter.

The criteria used by ALOHA for neutral-gas and dense-gas dispersion is as follows (Reynolds, 1992).

- $Ri_o \leq 1$ For neutral-gas dispersion
- $Ri_o > 1$ For dense-gas dispersion

It should be noted that an absolute threshold value does not actually exist. Dense-gas effects may begin to appear for Ri_o values less than one and become more pronounced as Ri_o is increased. It should also be noted that alternative definitions of Ri_o and corresponding dense-gas dispersion criteria are found in published literature (Hanna, 1996a).

Guidance for each parameter required by ALOHA for the direct source follows.

Source Strength Units

For the user's convenience, the source term may be entered on either a mass or volume basis. A variety of units (both metric and British) are available.

Source Duration

The source duration is specified as either instantaneous or continuous. A continuous release refers to any duration lasting longer than a minute. ALOHA assumes an instantaneous release to last one minute. Therefore, an instantaneous release is equivalent to a one-minute continuous release (e.g., specifying an instantaneous release of two kilograms is equivalent to specifying a continuous release of two kilograms per minute for a one-minute duration).

Recommendation: The recommendation below for source strength covers both source duration and source strength.

Source Strength

For an instantaneous release, the total quantity (mass or volume) released into the air is entered in the units specified by the source strength units chosen. For a continuous release the mass or volumetric release rate is specified as well as the duration in units of minutes. The allowable

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[17] Since D_o is not part of the input for the direct source, ALOHA does not have all the information to calculate Ri_o. For other source configurations D_o is either specified by user or calculated by ALOHA from the other input supplied.

input range for the duration is between 1 and 60 minutes. For the amount released, the allowable range is between 0 and 1,000,000,000, regardless of the units (NOAA, 1999b).

Recommendation: Conservatively specify release rate and duration. Calculated downwind concentrations are proportional to the release rate. So, the release rate should be conservatively estimated on the high side if there is some uncertainty or variability with its value. Note that for a given release rate, the calculated downwind concentrations generally increase as duration is increased (as the duration time increases, however, downwind concentrations become increasingly insensitive to further increases in duration).

Source Height

Only with the direct source may an elevated release be modeled, such as would occur with a stack discharge. A source height may specified for a neutrally buoyant (i.e., Gaussian dispersion) release. ALOHA will allow the user to specify a source height for a heavy gas, but the transport and dispersion calculations will be based on a ground level release.[18] This is consistent with the tendency of the heavy gas to slump to the ground.

Recommendation: The most conservative approach is to always assume a ground-level release. It is recommended, however, that the analyst use judgment based on site observation and published guidance to take credit for lower ground-level concentrations that can occur with elevated releases. Site observation is necessary since the elevated release from a stack can be negated by nearby structures. Releases from a stack can be drawn downward and entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs.

NRC Regulatory Guides 1.111 and 1.145 define a true "stack" release condition as one in which release occurs at or above 2.5 times the height of adjacent solid structures (NRC, 1977; NRC, 1983). It is recommended that the analyst enter the stack height only when this criterion is met of 2.5 times the height of adjacent structures. Otherwise, the release should be treated as ground level.

The identification of adjacent structures must take into account the extent of influence that the building has on the flow field in its vicinity. The wind flow that is directly over the top of the building is entrained downward into the wake cavity. The extent of the wake cavity downwind, as measured from the lee face of the building, can range from 2.5 times as great as the building height (H_b) to approximately 10 H_b for buildings that have large width-to-height ratios (Hanna, 1982). The wake cavity is marked by increased turbulence levels that decay progressively as a function of distance from the building. For releases from stacks not meeting the criterion of 2.5 times the height of adjacent solid structures, the combination of downward-directed entrainment into the wake cavity and increased dispersion due high turbulence levels serve to increase

[18] The output text will echo the source height that was entered even though the dense-gas transport and dispersion calculations were based on a ground-level release.

ground-level concentrations above what would be observed in the absence of the building. The term downwash is frequently used to collectively describe these effects. An accepted practice by the EPA is to assume that downwash effects can influence plumes that are released from stacks that are located in the range of 2 L upwind to 5 L downwind of building, where L is the lesser of the building height or projected width (EPA, 1995).

Physical State of Chemical

This input is only required when volume source strength units are chosen. Gas or liquid is entered to reflect the physical state of the stored chemical. ALOHA uses this input to convert the volume source strength to one of mass.

Chemical Storage Temperature

This input is only required whenever volume source strength units are chosen. ALOHA uses this input to convert the volume source strength to one of mass.

Recommendation: Usually chemicals are stored in tanks at ambient temperature. If the chemical is known to be stored at a different temperature, then that temperature should be entered.

Pressure of Stored Gas

This input is only required whenever volume source strength units are chosen, and the stored chemical is a gas. ALOHA uses this input to convert the volume source strength to one of mass.

Recommendation: When the user enters a pressure that is above ambient pressure, ALOHA responds with a warning that the user may want to consider modeling the scenario with either the tank or pipe source configuration models. Only a constant release rate can be considered with the direct source configuration. With the tank or pipe source configuration models, ALOHA will calculate a time-dependent release rate that takes into consideration the drop in source pressure that may occur as gas discharges from the tank or pipe.

<u>Puddle Source</u>

The puddle source algorithm is used when it is desired to calculate the time-dependent evaporation rate (non-boiling conditions) or vaporization rate (boiling conditions) of a known quantity of spilled chemical liquid that has pooled on the ground. Catastrophic failure of a storage vessel is an example of a scenario that could quickly progress to a puddle source configuration. The source term is proportional to the pool surface area, which is defined by the presence of a berm (or similar type barrier) or by assuming that the liquid spreads to some uniform thickness (e.g., 1 cm). As part of the source term solution, the mass and energy conservation equations are solved. The heat transfer mechanisms that are accounted for include short-wave solar influx, net longwave radiation flux between the pool and the atmosphere, ground-to-pool heat conduction, atmosphere-to-pool sensible heat flux[19], and latent heat flux[20] from evaporation or boiling vaporization (Reynolds, 1992) (Figure 4-3).

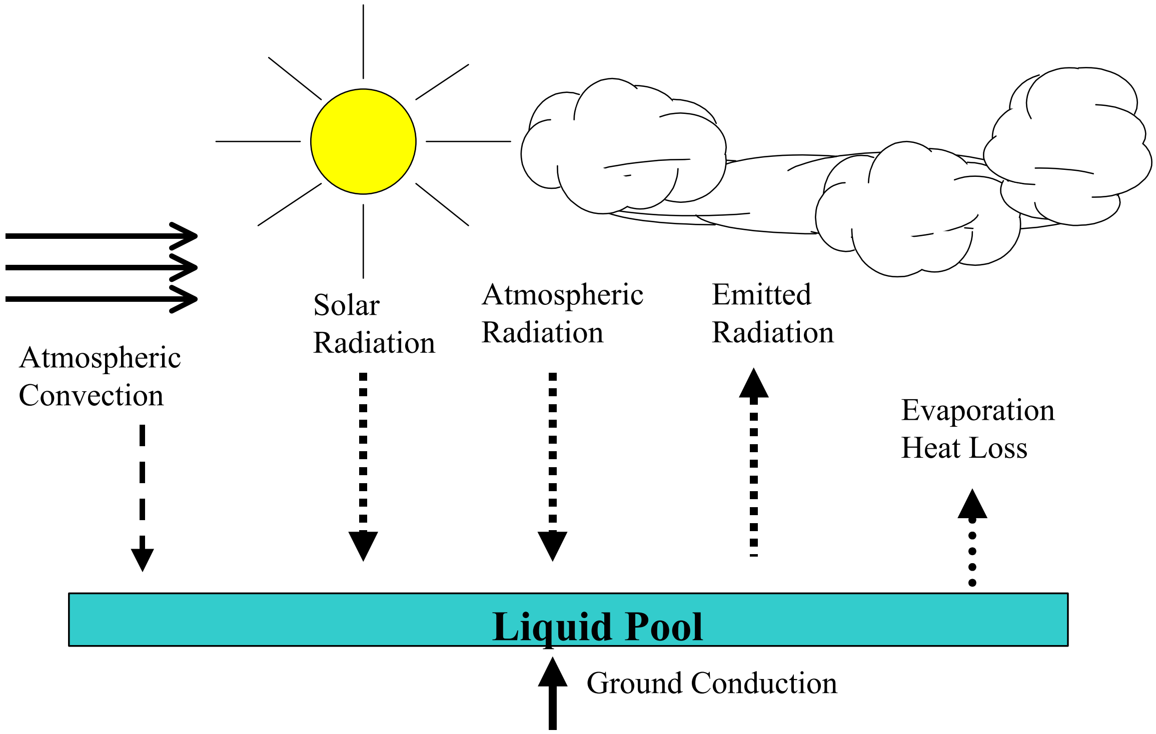

Figure 4-3. Heat Transfer Mechanisms with Puddle Source Configuration.

The Julian day, time of date, and global location (latitude and longitude) are inputs to the solar influx model (Raphael, 1962). The Stefan-Boltzman radiation law is the basis for the calculation of the net longwave radiation flux. The calculation of ground-to-pool heat flux uses the Fourier's law of heat conduction for transient, one-dimensional heat transfer of the pool in contact with a semi-infinite slab (representing the ground) of constant temperature (Carslaw, 1959). The pool temperature is assumed to be uniform. The analogy of mass transfer with heat transfer is the basis for the determination of the atmosphere-to-pool sensible heat flux. Brighton's steady-state solution of the advection-diffusion equation is the model for the evaporative mass transfer from the pool (Brighton 1985; Brighton, 1990). ALOHA assumes that the puddle grows thinner, while maintaining the same surface area, as the chemical material evaporates or boils. ALOHA considers all variables to be uniform throughout the puddle volume.

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[19] Sensible heat involves the release or absorption of thermal energy that is accompanied by a change in temperature.

[20] Latent heat is associated with phase change and involves the release or absorption of thermal energy with no change in temperature or pressure.

The liquid is non-boiling if the boiling point of the liquid (T_b) is greater than the ground temperature (T_g). The vapor pressure of the chemical at each time step determines the time-dependent evaporation rate (i.e., evaporative mass transfer) for non-boiling liquids and is a strong function of the puddle temperature (T_p). The sum of all the heat fluxes at each time step will either increase or decrease the internal energy of the puddle, and T_p will change proportionately to the change in internal energy.

If the boiling temperature of the liquid is less than the ground temperature, then the chemical vapor pressure is equal to the atmospheric pressure, and the liquid boils. The puddle temperature remains constant in time at the chemical boiling point. There is no change in the internal energy of the puddle as the evaporative heat flux balances the heat flux from the other heat flux sources. Thus, the net heat flux from these other sources at each time step determines the time-dependent vaporization rate. The term cryogenic refers to chemicals that have a very low boiling point, such that the ground-to-pool heat conduction is the dominant heat flux. ALOHA accounts for cooling of the ground beneath a cryogenic puddle.

Guidance for each parameter required by ALOHA for the puddle source follows.

Puddle Size I (Surface Area or Diameter)

This input (i.e., puddle surface area or diameter) and the next input (i.e., puddle volume, mass, or volume) together serve to characterize the quantity spilled and the physical dimensions of puddle that are necessary for evaporation calculations.

Either the surface area or diameter (for a circular puddle) is entered for the puddle-size I input. The input specification is straightforward if the spread of the puddle is constrained by the presence of the dike or similar structure that is being credited in the analysis. Topography can also play a role in confining the liquid to a certain area. For puddle that forms from an unconstrained spill,[21] one usually considers the total volume spilled and assumes spreading occurs to some minimum depth. In this case, a preliminary calculation must be first performed by the analyst to calculate the surface area or diameter given the volume and depth specifications. The basic equations are given below that relate the puddle diameter (d), surface area (A), volume (V) and depth (Δh).

$$A = V/\Delta h$$

$$d = (4/\pi \times A)^{0.5}$$

In the sample calculation that is presented in Section 7.0, these equations are used to calculate the surface area and diameter of the puddle that is consistent a the 210-gallon spill that spreads to a 1-cm depth.

[21] An unconstrained spill is analyzed when no barriers are present or have assumed to fail or when an unmitigated analysis is being performed in which no credit is being taken for the barriers that are present.

ALOHA assumes that the ground does not absorb any part of the spilled chemical. Moreover, the puddle diameter/surface area remains constant throughout the progression of the scenario (i.e., puddle grows thinner as liquid evaporates).

The allowable input range for the puddle area is between 20 square centimeters (3 square inches) and 31,400 square meters (37,500 square yards) (NOAA, 1999b). The allowable range for the puddle diameter is between 5 centimeters (2 inches) and 200 meters (220 yards) (NOAA, 1999b).

Recommendation: In an unmitigated analysis, no credit is taken for barriers and a puddle from an unconstrained spill is analyzed. Since the evaporation rate is proportional to the surface area, the analyst should make a conservative estimate of the maximum surface area or diameter that is reasonably conservative based on a maximum inventory and minimum puddle depth. The puddle-depth input is discussed below.

Puddle Size II (Volume, Mass or Depth)

This input in tandem with the puddle-size I input discussed above defines the total quantity of liquid spilled and completes the physical characterization of the puddle formed by a postulated spill. Either volume or mass (which equals the volume times the chemical liquid density) or depth (which equals the volume divided by surface area) is specified here.

The allowable input range for the volume is between 0.1 liter (0.026 gallon) and 10,000 cubic meters (2,640,000 gallons) (NOAA, 1999b). The depth must be between 1/4 centimeter (1/10 inch) and 100 meters (110 yards) (NOAA, 1999b). ALOHA accepts input values for mass between 1/10 kilogram (0.22 pound) and 100 metric tons (110 tons) (NOAA, 1999b).

Recommendation: It is recommended that a minimum depth of one centimeter be conservatively specified for an unmitigated spill analysis (EPA, 1987; Brereton, 1997).[22] As discussed above, the analyst should consider the maximum inventory in determining the volume spilled to form the puddle. This volume together with the one-centimeter depth should be used to calculate either the puddle surface area or puddle diameter that is needed for the puddle-size I input that is discussed above.

Ground Type

Ground type influences the amount of heat energy transferred from the ground to an evaporating puddle. ALOHA offers four choices for ground type:

- Default: unwetted soil not covered by rock or concrete

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[22] The 1-cm puddle depth is commonly used and suggested by EPA guidance (Brereton, 1997; EPA, 1987). Brereton (1997) notes that the 1-cm depth is somewhat arbitrary and recommends future development of an approach with more technical basis, such as one that would consider liquid physical properties (e.g., surface tension, viscosity) and ground surface properties (e.g., surface roughness).

- Concrete: concrete, cement, asphalt, or otherwise paved surfaces
- Sandy: sandy, dry soil
- Moist: sandy, moist soil

Recommendation: Heat is transferred most readily from a default or concrete ground into a puddle and least readily from sandy ground (NOAA, 1999b). The more heat energy that is transferred into the puddle, the higher the evaporation rate. The analyst should specify the ground type that most closely describes the area where the puddle has formed or choose a conservative ground type (e.g., default or concrete). If there is uncertainty or variability with the ground type, the user of course has the option of performing a parametric study on the sensitivity of the results to the ground-type input to aid in the specification of a conservative input.

Ground Temperature

The ground temperature also influences the amount of heat energy transferred from the ground to an evaporating puddle. The allowable input range for ground temperature is between -30 degrees C (-22 degrees F) and 64 degrees C (147 degrees F).

Recommendation: The best option is to make a specification based on statistical analysis of measurements of ground surface temperature (consistent with recommendation given in this document for air temperature). If these data are note available, the ground temperature should be set equal to the air temperature (Brereton, 1997; EPA, 1993).

Initial Puddle Temperature

The evaporation rate from a puddle is strongly dependent upon its temperature, increasing with increasing temperature. ALOHA assumes the initial temperature to be the uniform throughout the puddle volume (NOAA, 1999b). ALOHA accepts input that is between the liquid's freezing point and less than 9,937 degrees F (5,502 degrees C) (NOAA, 1999b). When the user specifies an initial puddle temperature that is above the normal boiling point of the liquid, ALOHA sets the temperature to the boiling point (NOAA, 1999b). It is expected that a boiling puddle will rapidly cool to its boiling point. ALOHA alert the user's that it is making this temperature adjustment.

Recommendation: The analyst should specify a liquid temperature that is consistent with the either the storage/operating temperature or the ambient temperature.

<u>Tank Source</u>

The tank source algorithm is used when it is desired to calculate the time-dependent source term when the chemical is stored in a tank that develops a leak. The chemical inventory of the tank can be a gas, liquid or liquefied gas.

- Gas Inventory: For gases, the time-dependent discharge rate from the tank is calculated using one-dimensional, compressible flow equations. The gas discharge rate quantifies the source term and is primarily a function of storage pressure and hole characteristics (size, shape, and location). The flow is either choked or unchoked at each time step depending upon the ratio of the tank pressure to atmospheric pressure and the critical pressure ratio for sonic flow. ALOHA takes into account the reduction in driving pressure and the temperature drop that occurs due to adiabatic expansion as the gas leaves the tank. ALOHA assumes that the heat flux through the tank walls has a negligible effect on the gas temperature. If the leak is through a short pipe or valve connect to the tank, frictional losses are neglected, simplifying the problem to that of a leak through an orifice-like hole in the tank. The leak stops once the pressure in the tank reaches atmospheric (i.e., enough gas is left in the tank to maintain atmospheric pressure).

- Liquid Inventory: Liquids leak from a tank at a time-dependent rate that is proportional to the size of the hole and described by Bernoulli's equation. The driving pressure is the sum of the vapor space pressure (set equal to the vapor pressure of the chemical) and the hydrostatic pressure of the column of liquid above the hole. The discharge coefficient is set to a value of 0.61 (Reynolds, 1992). As liquid leaves the tank, liquid evaporates or air ingested to maintain the vapor space pressure (Evans, 1993). Liquid leaks until the liquid level in the tank drops below the level of the hole. The temperature in the tank at each time step changes due to the net effect of evaporative heat loss and heat transfer through the tank walls.[23] The liquid that discharges from the tank falls to the ground to form a pool that may initially grow in size depending upon the evaporation or vaporization rate in comparison to the liquid discharge rate. ALOHA allows a minimum depth of 0.5 cm to be achieved and restricts spreading to maintain this minimum depth while spreading occurs (NOAA, 1999b). The puddle spreads until the evaporation rate or vaporization rate balances the spreading rate. At this point, the puddle surface area remains constant and grows thinner (0.5-cm minimum depth no longer imposed) as the chemical material evaporates or boils, consistent with the algorithms for the puddle source configuration. The puddle-source algorithms are the basis for determining the time-dependent rate at which the chemical evaporates or boils. The puddle energy balance includes an additional term that accounts for the energy due to any temperature difference between the liquid entering the puddle from the tank and the puddle itself.

- Liquefied Gas Inventory: The term "liquefied gas" refers to a chemical substance that is a vapor at atmospheric pressure and temperature, but is stored as a liquid. The chemical substance in storage may be either cooled (i.e., refrigerated) at ambient pressure or pressurized (i.e., compressed) at ambient temperature to achieve and maintain the liquid state. The refrigerated liquefied gas situation is conceptually straightforward and the easier of the two situations to model. A refrigerated liquefied gas is modeled as a liquid discharging from tank that forms a boiling puddle on the ground.

[23] ALOHA assumes 1-cm thick steel walls.

The model for the compressed liquefied gases must consider additional phenomena that can be quite complex. The various phenomena that may occur are briefly discussed followed by a discussion of the simplifications that ALOHA applies to the problem. Compressed liquefied gases may change from the liquid to vapor state in the tank as the pressure drops (i.e., flash boiling), at the exit from the tank in the form of a jet spray (i.e., two-phase flow), or on the ground through boiling. All three vapor-forming mechanisms may occur in one accident. Flash boiling (or flashing) occurs as the sudden depressurization results in the tank liquid being temporarily in the superheated condition (i.e., with excess latent heat as a result of being a liquid at a temperature above its boiling point). The internal excess heat rapidly vaporizes the liquid to vapor. The flashed vapor rapidly expands and fragments surrounding liquid into fine droplets that create a foam mixture that fills the tank. The greater the superheat, the smaller the diameter of the liquid droplets. Liquid droplets that leave the tank in the jet-spray discharge may turn to vapor through flash boiling (as jet expansion outside the tank results in a further pressure reduction) or through general boiling as the atmospheric air externally exchanges energy with the droplet. If any liquid reaches the ground, a boiling puddle will form on the ground. ALOHA conservatively assumes, however, that all droplets leaving the tank are vaporized, so that no puddle is formed (only vapor and droplets that vaporize before reaching the ground exit the tank).

In calculating the mass discharge rate, ALOHA uses different algorithms to model the jet-spray discharge depending upon whether the leak is a simple hole in the tank or is at the end of a short length of pipe. In each case, ALOHA assumes that the tank contents form a uniform two-phase mixture.[24] For a simple hole, ALOHA uses a modified version of Bernoulli's equation in which the uniform two-phase mixture assumption is used to determine of the hydrostatic pressure. The density of the two-phase mixture is conservatively based on the liquid density, resulting in an over-estimation of the mass discharge rate. For a short pipe, the mass discharge rate is based on homogeneous nonequilibrium and homogeneous equilibrium models (Henry, 1971; Fauske, 1985; Leung, 1986; Fauske; 1988). The length of pipe is set to 0.1 m, which is conservative for longer pipes since mass discharge rates decrease slightly with increasing pipe length.[25] ALOHA tracks the amount of liquid and vapor remaining in the tank after each time step, and the leak stops once the pressure in the tank reaches atmospheric and hydrostatic pressure has dropped to zero (liquid level has reached bottom of hole) (Evans, 1993). The temperature in the tank is set at or above the boiling point at each time step (ALOHA considers the net effect of vaporization heat loss and heat transfer through the tank walls at each time step).

Guidance for each parameter required by ALOHA for tank source follows.

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[24] The uniform two-phase mixture completely fills the tank unless the criterion set by ALOHA for the maximum allowable quality (ratio of mass of vapor to total mass) is exceeded.

[25] The choice of 0.1-m pipe length is judicious since the homogeneous nonequilibrium model approximately reduces to the homogeneous equilibrium model as the length of the pipe approaches 0.1 m. It should also be noted that the homogeneous nonequilibrium model with zero pipe length reduces to the modified Bernoulli's equation that is used in ALOHA for the simple hole case (Reynolds, 1992).

Tank Type/Orientation

ALOHA models three tank types.

- Horizontal cylinder
- Upright cylinder
- Sphere

Recommendation: Choose the type that best approximates the type of tank being analyzed.

Tank Size

For a sphere, the diameter or volume of the tank is to be entered. Here, volume refers to the total capacity of the tank and not to the volume of chemical in the tank. For a cylinder, values for two of the following three parameters are to be entered: diameter, length, and volume. ALOHA will compute and display values for the remaining dimension not entered for the sphere or cylinder. The allowable range for tank diameter is between 20 centimeters (about 0.7 feet) and 1,000 meters (3,280 feet) (NOAA, 1999b). Tank length must be between 50 centimeters (about 1.7 feet) and 1,000 meters (3,280 feet) (NOAA, 1999b).

Physical State of Chemical

ALOHA provides three input options for physical state of the chemical.

- Tank contains liquid
- Tank contains gas only
- Unknown

ALOHA uses this input to support the determination of the quantity of chemical in the tank and its rate of discharge from the tank.

Recommendation: ALOHA provides the following guidance (NOAA, 1999b).

- Tank contains liquid – appropriate if there is any liquid in the tank, even if it's just a small amount
- Tank contains gas only – appropriate when the tank contains only gas, with no liquid present
- Unknown – appropriate when uncertain about physical state of the chemical

Mass of Chemical in Tank

This input is only required if the physical state of the chemical is unknown. ALOHA uses this input along with the temperature input (discussed next) and the chemical properties to determine the physical state of the chemical. The mass entered must be greater than zero but less than 100,000 tons (200,000,000 pounds or 90,720,000 kilograms) (NOAA, 1999b).

Recommendation: Since the liquid discharge rate increases with increasing mass, the mass should be conservatively estimated on the high side if there is some uncertainty or variability with its value.

Chemical Storage Temperature

The storage temperature of a chemical within a tank determines its physical state (gas, liquid, or solid) and the pressure within the tank. These variables are important factors in estimating the rate of discharge from the tank.

If the chemical is identified as a gas and the temperature entered is below the chemical's normal boiling point, ALOHA will tank respond with a warning that the chemical is not a gas. The user should then consider that the chemical is in the liquid state if a check verifies that the correct inputs have been entered.

ALOHA will alert the user if storage temperature entered exceeds both the chemical's boiling point and the ambient air temperature. This warning, however, will not impede the analysis. The allowable input range is between than -459 degrees F (-273 degrees C) and 9,937 degrees F (5,503 degrees C) (NOAA, 1999b).

Recommendation: Usually chemicals are stored in tanks at ambient temperature. If the chemical is known to be stored at a different temperature, that temperature should be entered.

Mass or Pressure of Stored Gas

This input is only required if the physical state of the chemical is a gas. The input will take one of three forms.

- Tank pressure
- Mass of gas in the tank
- Volume of gas in the tank at standard temperature and pressure

If the pressure is entered, ALOHA will calculate the mass (or volume) and show its value in the space reserved for the mass (or volume) input in the dialog box.

ALOHA also checks to ensure that the chemical is a gas based upon the inputs of tank size, chemical storage temperature, and tank pressure (or equivalently chemical mass or volume). If the tank pressure is not high enough to liquefy the gas, ALOHA will respond with a warning that the chemical is not a gas. The user should then consider that the chemical is in the liquid state if a check verifies that the correct inputs have been entered.

The mass entered must be greater than zero but less than 10,000 tons (20,000,000 pounds or 9,720,000 kilograms) (NOAA, 1999b). The allowable input range for pressure is between 1.1 atmospheres (836 millimeters of mercury, 16.2 pounds per square inch, or 111,458 pascals) and 68 atmospheres (51,680 millimeters of mercury, 1,000 pounds per square inch, or 6,890,100 pascals) (NOAA, 1999b). The pressure must be at least 1.1 atmospheres for ALOHA to calculate any gas release from the tank (NOAA, 1999b). The release stops once the pressure in the tank reaches atmospheric (i.e., not all the gas leaves the tank as some remains in the tank to maintain atmospheric pressure inside).

Recommendation: Since the gas discharge rate increases with increasing pressure (or mass), the pressure (or mass) should be conservatively estimated on the high side if there is some uncertainty or variability with its value.

Mass or Volume of Stored Liquid

This input is only required if the physical state of the chemical is a liquid. The input will take one of three forms.

- Mass of liquid and vapor in the tank
- Volume of liquid in the tank
- Percent of tank volume that is filled with liquid

After an entry is made for one of the above parameters, ALOHA calculates values for the other two parameters and displays their values in the dialog box.

The mass entered must be greater than zero but less than 10,000 tons (20,000,000 pounds or 9,720,000 kilograms) (NOAA, 1999b). The volume cannot exceed the tank capacity nor can the percent full exceed 100%.

Recommendation: Since the liquid discharge rate increases with increasing mass (or volume of liquid), the mass (or volume of liquid) should be conservatively estimated on the high side if there is some uncertainty or variability with its value.

Shape of Leak Opening

ALOHA offers the choice of rectangular opening or circular opening.

Recommendation: Choose the shape that best approximates the opening that is postulated for the scenario.

Size of Leak Opening

The diameter is to be entered for a circular opening and the length and width for a rectangular opening. The diameter of a circular opening must be at least 0.1 centimeter (0.04 inch) (NOAA, 1999b). The length of a rectangular opening must be at least 1 centimeter (0.4 inch) and its width must be at least 0.1 centimeter (0.04 inch) (NOAA, 1999b).

The area of the opening must less than the circular cross-sectional area of the tank or 10% of the total tank surface area, whichever is smaller (NOAA, 1999b). If the rupture area is larger than this, then the release must be modeled as a direct source or puddle source as directed below (NOAA, 1999b).

- The direct-source configuration is to be used with a gas inventory or if the tank is pressurized and a two-phase discharge is expected, such as the case with a liquefied gas inventory. The total chemical mass should be instantaneously released.

- The puddle-source configuration should be used with a liquid inventory. The total chemical mass should comprise the puddle.

Recommendation: Since the liquid or gas discharge rate increases with increasing leak size, the leak size should be conservatively estimated on the high side if there is some uncertainty or variability with this input.

Type of Leak Opening

ALOHA offers the choice of a leak through a hole opening directly in the tank wall or through a short pipe or valve that extends at least 10 centimeters (4 inches) from the wall of the tank.

Recommendation: Hole type does not make a difference for a pure-gas discharge or for a pure liquid leak (NOAA, 1999b). For the liquefied gas release, ALOHA accounts for the friction generated as the two-phase mixture of liquid and gas flows through the valve or short pipe. As a result, higher release rates are calculated with the hole opening. The hole opening is thus recommended for conservative results unless the case for the valve or short-pipe opening can be adequately defended for the postulated scenario.

Height of Leak Opening

This input is not required if the physical state of the chemical is a gas. ALOHA allows this input to be expressed as either the distance from the tank bottom or percent way up to the top of the tank (once a value is entered for one of these parameters, ALOHA calculates the value for the other parameter and displays it in the dialog box).

For a pure liquid release, ALOHA uses this input to determine whether or not the hole site is above or below the liquid level in the tank. Liquid will spill from the hole until enough liquid drains from the tank to drop the liquid level below the hole (NOAA, 1999b). Liquid that spills to the ground forms a pool.

Recall that for the liquefied gas case, ALOHA assumes that a uniform two-phase mixture fills the tank (Reynolds, 1992). A mixture gas and droplets leave the tank, but the droplets are assumed to evaporate before reaching the ground (i.e., no puddle forms) (Reynolds, 1992). In general, the leak stops once the pressure in the tank drops to atmospheric and hydrostatic pressure has dropped to zero (liquid level has reached bottom of hole) (Evans, 1993). If the hole is at the bottom of the tank, however, the entire mass of the inventory is assumed to exit the tank (i.e., even the mass that would be expected to remain in the tank once the pressure reached atmospheric is conservatively assumed to exit the tank) (Evans, 1993).

Recommendation: The quantity of liquid that spills to form a puddle on the ground for the pure liquid case increases with lower leak opening heights, which results in higher evaporation rates for a puddle that forms from an unconstrained spill. Moreover, the hydrostatic pressure, which increases with increasing distance between the liquid surface and the hole, establishes the driving force for the discharge rate. Therefore, the height of the leak opening should be conservatively estimated on the low side if there is some uncertainty or variability with its value. The same approach of conservatively estimating the height of the leak opening on the low side should also be used for the liquefied gas case even though different phenomena come into play.

Surface Ground Type and Temperature

This input is only required if the physical state of the chemical is a liquid. For a liquid spill, a puddle will form on the ground, and ALOHA will calculate the evaporation rate from the puddle.

Recommendation: Follow the guidance given for the puddle source.

Maximum Puddle Diameter or Area

This input is only required if the physical state of the chemical is a liquid. Like for the puddle source, the specification is straightforward if the spread of the puddle is constrained by the presence of the dike or similar structure that is being credited in the analysis. When the spill is assumed to be unconstrained for the tank discharge case, ALOHA offers the option of choosing "unknown" for the maximum puddle diameter or area. ALOHA assumes that an unconstrained puddle will spread until the depth reaches 0.5 cm (about 0.2 inch). Note that this is conservative with respect to the recommended value of 1.0 cm given above for the unconstrained spread of a puddle source.

The allowable input range for the puddle area is between 20 square centimeters (3 square inches) and 31,400 square meters (37,500 square yards) (NOAA, 1999b). The allowable range for the puddle diameter is between 5 centimeters (2 inches) and 200 meters (220 yards) (NOAA, 1999b).

Recommendation: Follow the guidance given for the puddle source and letting the puddle spread unconstrained for unmitigated accident analysis.

Pipe Source

The pipe source configuration represents gas discharges from a long pipe either (i) connected to a large-capacity reservoir (ii) closed off at its unbroken end.[26] The length-to-diameter ratio of the pipe must be at least 200 (if not, an ALOHA warning suggests that analyst use the tank source configuration). ALOHA assumes that the flow of gas through the pipe is isothermal, except for the last 200 pipe diameters. A balance between frictional heating and expansion cooling will result in isothermal flow. Gas moving through the last section of pipe is expected to expand adiabatically. Based on the user input of either rough or smooth for the inside walls of the pipe, ALOHA calculates a friction factor. The rupture area may be a size up to the cross-sectional area of the pipe.

ALOHA models the initial flow as choked for both cases of a large-reservoir source and a closed-off source. The initial flow rate is a function of rupture area, initial pressure, initial temperature, and the specific heat ratio of the gases. The flow is essentially steady for the large-reservoir source. For the closed-off source, the pressure will drop and the mass flow rate is reduced as gas empties from the pipe.

Guidance for each parameter required by ALOHA for the puddle source follows.

Pipe Diameter

ALOHA uses the inside pipe diameter to predict the discharge rate from a ruptured pipeline. The allowable input range is between 1 centimeter (0.4 inches) and 10 meters (32.8 feet) (NOAA, 1999b).

Recommendation: Since the gas discharge rate increases with increasing pipe diameter, the pipe diameter should be conservatively estimated on the high side if there is some uncertainty or variability with this input.

Pipe Length

ALOHA uses the pipe length to predict the discharge rate from a ruptured pipeline. The allowable input range is between 200 times the pipe diameter and 10 kilometers (6.2 miles) (NOAA, 1999b). If the pipe is shorter than 200 times its diameter, then the analyst should consider modeling the release using the tank source configuration.

Recommendation: Since the gas discharge rate increases with decreasing pipe length, the pipe length should be conservatively estimated on the low side if there is some uncertainty or variability with this input.

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[26] The pipe source configuration does not support liquid discharges from pipes. In some instances, it may be possible to model liquid releases from a pipe using the tank source configuration, given that the pipe diameter is at least 8.4 inches (20 centimeters) and the length is no longer than 3,280 feet (1000 meters) (NOAA, 1999a).

Pipe Scenario (Unbroken End State)

ALOHA can model two different types of scenarios for a gas pipeline leak. The two types of scenarios differ in the state of the unbroken end.

- The unbroken end is closed off (e.g., shut-off valve), so a finite amount of gas is in the pipeline section. As gas is discharged at the broken end, the pressure drops and the discharge rate slows over time. The release occurs over a finite period of time

- The unbroken end is connected to a very large, essentially infinite, reservoir. Pressure and discharge rate remain essentially constant, and the release occurs for an indefinite period of time.

Recommendation: Use the model that best describes the scenario that is being analyzed.

Pipe Roughness

ALOHA uses the pipe surface roughness to predict the discharge rate from a ruptured pipeline. The rougher the pipe, the more friction as the gas flows through the pipe. Friction creates energy losses that result in lower discharge rates. ALOHA offers the two choices of surface roughness under the labels of smooth pipe and rough pipe. Examples of a rough pipes are those that have inner surfaces that have rusted or been corroded. Smooth pipes include new metal pipes, glass pipes and plastic pipes.

Recommendation: Since the gas discharge rate is higher with a smooth pipe, the smooth pipe should be conservatively used if there is some uncertainty or variability with this input.

Pipe Pressure

ALOHA uses the pipe pressure to predict the discharge rate from a ruptured pipeline. The allowable input range is between twice the ambient air pressure and 680 atmospheres (10,000 pounds per square inch) (NOAA, 1999b).

Recommendation: Since the gas discharge rate increases with increasing pipe pressure, the pipe pressure should be conservatively estimated on the high side if there is some uncertainty or variability with this input.

Temperature of Chemical in the Pipe

ALOHA uses the temperature of the chemical in the pipe to predict the discharge rate from a ruptured pipeline. The allowable input range is between the boiling point of the chemical and 1,535 degrees C (2,795 degrees F) (NOAA, 1999b).

Recommendation: ALOHA recommends that the temperature be set to the ambient temperature if unknown (NOAA, 1999a; NOAA, 1999b). This seems reasonable, especially when one considers that the results are not expected to be real sensitive to the temperature input. The user always has the option of performing a parametric study on the effect of chemical temperature to aid in the specification of a conservative input.

Hole Size

ALOHA uses the hole size to predict the discharge rate from a ruptured pipeline. This input is only required for the scenario involving the closed-off unbroken end. For the scenario involving the infinite reservoir, ALOHA assumes that the pipe is completely sheared off, such that the hole diameter equals the pipe diameter. For scenario involving the closed-off unbroken end, an area for the hole can be specified up to the area corresponding to the pipe diameter.

Recommendation: Since the gas discharge rate increases with hole size, the pipe pressure should be conservatively estimated on the high side if there is some uncertainty or variability with this input.

4.3.4 COMPUTATIONAL PREFERENCES

Under the computational preferences, ALOHA allows a couple of miscellaneous options that affect the computations to be changed from default values.

Dispersion Model

ALOHA presents three choices.

- Let model decide (default condition)
- Use Gaussian dispersion only
- Use heavy gas dispersion only

ALOHA generally makes a determination of whether the heavy gas dispersion model is to be used on the basis of the source Ri number has discussed previously. In order to calculate the source Ri number, the following chemical property data are required (NOAA, 1999b).

- Chemical name
- Molecular weight
- Normal boiling point
- Gas density, with a reference temperature and pressure
- Gas heat capacity (constant pressure), with a reference temperature and pressure
- Critical temperature and pressure or vapor pressure at 1 atmosphere with a reference temperature

If any of the above items are missing in the database library for the chemical of interest, ALOHA will calculate downwind concentrations using the Gaussian dispersion model.

Recommendation: The analyst generally should allow the ALOHA algorithms to determine which dispersion model to use (default condition). As stated above, ALOHA generally makes this determination on the basis of the source Ri number. Assuming the chemistry property data listed above is available in the database library, ALOHA has the information to calculate the source Ri number for the puddle, tank, and pipe source configurations. ALOHA cannot calculate the source Ri number for the direct source configuration, however, since the necessary length scale or area dimension is not supplied. For the direct source configuration, ALOHA apparently makes a determination solely on the molecular weight of the gas or vapor released. It is better if the analyst calculates the source Ri number when using the direct source configuration and then chooses the appropriate dispersion model. This is the recommended approach. In some cases, the analyst may judge it appropriate to calculate results with both models and use the more conservative of the two sets of results.

Dose Exponent

ALOHA defines the dose as "the concentration of pollutant at a specified location (to which people may be exposed), taken to a power, and multiplied by the period of time that it is present." The power "n" in this definition is referred to as the dose exponent.

Recommendation: For accident analysis work, human health evaluation guidelines, such as ERPGs and TEELs, are based on concentration limits and not dose limits. Therefore, doses calculated by ALOHA are not used. The ALOHA documentation states that its dose results are of limited use and only for use by someone trained in toxicology. The following is an excerpt from the user's manual and online help (NOAA, 1999a; NOAA, 1999b).

> *Dose information is difficult to interpret because the effects of most toxic chemicals on people are poorly understood. If you don't know the appropriate dose exponent to use for a particular chemical, or can't consult with a specialist who can advise you on the correct exponent to use and help you to interpret ALOHA's results, AVOID USING ALOHA'S DOSE CALCULATIONS. Instead, use information from ALOHA's footprint and concentration plots and your own knowledge of a chemical to make response decisions.*

4.4 Input Recommendations for Display Parameters

In general, the submenus that are included under the Display menu are concerned with the output options that are largely a matter of personal preference. An input of technical importance to the analysis, however, is found in the Options submenu. Here, an ERPG or TEEL value can be entered as the LOC value.

Options (TEEL or ERPG input)

The American Industrial Hygiene Association (AIHA) has issued three levels of ERPG values based on toxic effect of the chemical for use in evaluating the effects of accidental chemical releases on the general public (AIHA, 2002). The ERPGs are estimates of concentrations for specific chemicals above which acute exposure (up to 1 hour) would be expected to lead to adverse health effects of increasing severity for ERPG-1, ERPG-2, and ERPG-3. The definitions of each ERPG level in terms of toxic effects are as follows (AIHA, 2002).

> ***ERPG-1****: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing more than mild, transient health effects or without perceiving a clearly defined objectionable odor.*
>
> ***ERPG-2****: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing irreversible or serious health effects or symptoms that could impair an individual's ability to take protective action.*
>
> ***ERPG-3****: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.*

Like the ERPGs, the TEELs are a collection of chemical-specific concentrations corresponding to varying levels of health effects (Craig, 2001). TEELs have been developed since ERPGs are available for only a limited number of chemicals. The TEELs are comprised of (a) Emergency Response Planning Guideline (ERPG) values for all chemicals for which ERPGs have been published and surrogate ERPG values for chemicals for which ERPGs have not been published (i.e., the TEEL-1, -2, and -3 values), and (b) Permissible Exposure Limit - Time-Weighted Average (PEL-TWA) values for all chemicals for which PEL-TWA values have been published and surrogate PEL-TWA values for chemicals for which PEL-TWA values have not been published (i.e., the TEEL-0 values) (Craig, 2001). PEL-TWA values are developed by the Occupational Safety & Health Administration (OSHA) for use in limiting worker exposures to airborne chemicals (CFR, 1999). Most people are not expected to experience any adverse health effects to accident exposures at the TEEL-0 level (Craig, 2001).

Recommendation: The DOE has not provided definitive evaluation guidelines for chemical exposures, so the specific use of ERPGs and TEELs in accident analysis remains an open issue. It is recommended that guidance from subject-matter experts be followed (Craig, 2001).

5.0 SPECIAL CONDITIONS FOR USE

ALOHA is a public domain code that is part of a system of software that is known as the Computer-Aided Management of Emergency Operations (CAMEO) that was developed to plan for and respond to chemical emergencies. This document does not address applications related to emergency response or emergency preparedness/planning.

Even though ALOHA was not developed specifically for safety analysis applications, it is also widely used throughout the DOE complex for this purpose and part of the toolbox codes that have been identified by DOE to support 10 CFR 830 safety analysis. This document serves as a guide for acceptable implementation of the ALOHA code for the purpose of modeling source term and consequence phenomenology in the context of supporting safety basis documentation

6.0 SOFTWARE LIMITATIONS

The limitations of a computer code must be discussed in the context of its intended use. The limitations of ALOHA that are discussed in Table 6-1 below relate to both its use in general and specifically for safety analysis applications (recall that ALOHA was developed to plan for and respond to chemical emergencies).[27]

6.1 ALOHA Issues

Table 6-1 ALOHA Limitations

ALOHA Limitation	Comment
Results are less reliable for conditions of low wind speed or very stable atmospheric conditions.	Issue of general concern to atmospheric transport and dispersion codes.
Results have high uncertainty very close to the source.[28]	Issue of general concern to atmospheric transport and dispersion codes. ALOHA shows average concentrations that are based on laws of probability and meteorologists' knowledge of atmospheric phenomena (NOAA, 1999a).

[27] Differences exist in the computational capabilities that are needed for a safety analysis calculation compared to those that are needed by people responding to a chemical accident. For example, the direction that a chemical puff or plume is travelling is of utmost importance to an emergency responder, since this information is crucial if efficient evacuation procedures are to be implemented. Thus, the inability of ALOHA to allow for shifts in wind direction during the course of modeling an accidental chemical release is a code limitation that affects emergency response calculations. Safety analysis calculations, however, traditionally consider exposures to a hypothetical receptor that is stationed on the centerline of a plume that is invariant with time. Thus, the inability of ALOHA to model shifts in wind direction does not constitute a limitation in the context of safety analysis calculations.

[28] In some cases, ALOHA may actually calculate an outdoor concentration near the source of greater than 1,000,000 parts per million, which is physically impossible. Substances that are gases at ambient temperature and pressure have an ambient saturation concentration of 1,000,000 parts per million, or 100%. The following text is from a 5/20/1999 e-mail from ALOHA technical support that is related to this topic:

> When using the direct source option, ALOHA does not simulate the effects of jets, or high pressure releases, rather it assumes that the dispersion is dominated by turbulent diffusion in the atmosphere. Depending on the specifics of the release, pressure driven diffusion may well dominate the near field region. The ALOHA direct source option starts with a point source containing all the pollutant and allows it to diffuse as it travels downwind. This model should not be interpreted as a representation of reality close to the source where pressure effects, jets, and near-field patchiness play significant roles. Close to the source ALOHA artificially compresses all the pollutant into a small volume (even using the ideal gas law, it should be obvious that as the volume shrinks, the

Table 6-1 ALOHA Limitations (continued)

ALOHA Limitation	Comment
ALOHA does not allow for one or more years of meteorological data to be input and processed so that statistical methods can be employed to determine the 50th percentile (median) or 95th percentile (unfavorable) concentration results.	ALOHA accepts a single input combination of atmospheric stability class and wind speed. The user is responsible for specifying an appropriate combination of atmospheric stability class and wind speed that will yield representative median or unfavorable concentration results. If one or more years of meteorological data are available, other atmospheric dispersions that can accept and process the meteorological data can be used to assist in these specifications. For example at SRS, meteorologists evaluated SRS data with another atmospheric and dispersion code for neutrally buoyant plumes and found that the 95th percentile conditions were associated with E stability class and 1.7-m/s wind speed for ground level releases (Hunter, 1993). Alternatively, an electronic worksheet may also be programmed to perform similar analysis. In lieu of site-specific meteorology, the accident analysis may use generally accepted, default stability and wind speed combinations. For example, F stability class and 1.5 m/s wind speed is recommended by the EPA for analysis of ground-level releases of neutrally buoyant plumes (EPA, 1996). For dense gas releases, sensitivity studies are recommended to determine median and unfavorable meteorological conditions.
ALOHA does not model the initial momentum of the release.	ALOHA does not account for the initial plume rise from momentum effects. This approach is conservative in accident analysis applications since the ground-level concentration will be less with an elevated release with respect to a ground-level release when plume depletion from deposition effects are ignored, as is done in ALOHA.

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concentration get large). Obviously, when the reported mole fraction in the air is over 100% you are too close to the source for the model to be trusted.

Table 6-1 ALOHA Limitations (continued)

ALOHA Limitation	Comment
ALOHA does not account for the effects of fires or chemical reactions.	ALOHA does not account for the initial plume rise from buoyancy effects. This approach is conservative in accident analysis applications since the ground-level concentration will be less with an elevated release with respect to a ground-level release when plume depletion from deposition effects are ignored, as is done in ALOHA. Also, ALOHA does not model combustion or chemical reactions of any kind. When the user selects an air- or water-reactive chemical, ALOHA informs the user of the type of reaction and expected reaction products. For example, sulfur trioxide reacts with water to form sulfuric acid and heat. ALOHA does not account for resulting phenomena such as buoyancy from the heat. Specialty codes have been developed to consider scenarios in which modeling specific chemical reactions is important in assessing toxicological effects. For example, HGSYSTEM/UF6 has been developed to model releases of UF_6 from containers and the chemical and thermodynamic processes that result from interaction of uranium hexaflouride (UF_6) with water vapor in the air to form hydrogen flouride (HF) (Hanna, 1996b).
ALOHA does not account for terrain steering effects.	A natural canyon or street canyon formed by large buildings can constrain the lateral dispersion of the puff or plume. Development of codes that are suitable for complex terrain and urban settings is an area of ongoing research.
ALOHA does not model dispersion effects associated with building wakes.	Since wake effects near the source tend to enhance dispersion that provides additional dilution, it is generally believed to be conservative to neglect these effects in estimating chemical concentrations at downwind locations for ground-level releases.

Table 2-1 ALOHA Limitations (continued)

ALOHA Limitation	Comment
ALOHA does not model the evaporation of chemical constituents in a mixture or solution.	The property information for chemicals in the ALOHA database is limited to pure chemicals. The vapor pressure of the chemical is a key parameter in establishing the evaporation rate. For a chemical constituent in solution, the vapor pressure of the chemical constituent is a function of its concentration and temperature. The chemical database does allow new chemicals and their properties to be added to the database. In some versions of ALOHA (such as 5.2.3), the vapor pressure can be entered directly (along with the reference temperature for the vapor pressure value) or calculated on the basis of other input properties, namely, the boiling point, freezing point, critical pressure, and critical temperature.[29] Actual data for these properties for chemical constituents in solution are rare, however, especially data for critical pressure and critical temperature. While ALOHA accepts the direct input of vapor pressure, it still requires the above-mentioned property data for sources other than the direct source configuration (NOAA, 1999a). An approach has been used with success at Savannah River Site (SRS) for dilute acids (e.g., 70 weight percent nitric acid) that involves entering pseudo property values for the boiling point, freezing point, critical pressure, and critical temperature. These pseudo property values are set through trial and error so that the ALOHA chemical database calculates vapor pressures at the temperature range of interest that closely match the vapor pressures for the dilute acid as found in a reference book. The sample calculation in Section 7.0 includes evaporation rate calculations for nitric acid for both 100 weight percent and 70 weight percent solutions.

[29] ALOHA also uses these properties to calculate liquid and gas density.

Table 2-1 ALOHA Limitations (continued)

ALOHA Limitation	**Comment**
ALOHA limits predictions to one hour after the release begins or to distances up to ten kilometers (6 miles).	With a wind speed of approximately 2.8 m/s, the puff or plume will travel a distance of approximately 10 km. The downwind extent of the puff or plume will be less for lower wind speeds. For example, the puff or plume will travel a distance of approximately 5.4 km for a wind speed of 1.5 m/s, which is commonly used for worst-case consequence calculations. Therefore, ALOHA is incapable of making concentration predictions for receptors beyond approximately 5.4 km for a wind speed of 1.5 m/s. Of course, if the concentration is less than the LOC concentration at the maximum computed ALOHA distance, the concentration will be even lower and below the LOC at distances even farther away. If concentrations need to be calculated beyond the maximum computed ALOHA distance, the analyst may have to perform a hand calculation using the Gaussian model for either a plume (Equation A-1) or a puff (Equation A-4). At these distances, the Gaussian model is appropriate since enough air has mixed with the puff or plume for it to be neutrally buoyant even if it started out as a dense-gas cloud.
ALOHA does not model processes that affect the dispersion of particles, such as deposition from gravitational settling	In the case of low concentrations of airborne particles, it is reasonable to neglect transport phenomena peculiar to particulate and to assume that the particles act as a passive scalar contaminant that follows the flow field (Hanna, 2002). Larger particles released in a puff or plume will fall to the ground due to gravitational settling. Smaller particles and even gases will deposit on ground surface elements (e.g., ground vegetation) through a process known as dry deposition. Dry deposition refers to chemical reactions and physical interactions between the contaminant (particle or gas) in the puff or plume and the ground surface elements that serve to

	remove the contaminant from the puff or plume.

6.2 Outcome of Gap Analysis

To be added at a later date.

7.0 SAMPLE CALCULATIONS: PUDDLE EVAPORATION

Problem Statement: A vessel at SRS (Aiken, SC) stores 210 gallons of concentrated (> 90 wt%) nitric acid (HNO_3) at ambient pressure and temperature. A scenario is postulated in which the vessel ruptures catastrophically, and the 210 gallons of HNO_3 spill on the ground. Determine the following: (1) the maximum concentration at 100 meters downwind and compare with the ERPG-3 value of 78 ppm and (2) the maximum concentration at 2500 meters downwind and compare with the ERPG-2 value of 6 ppm.

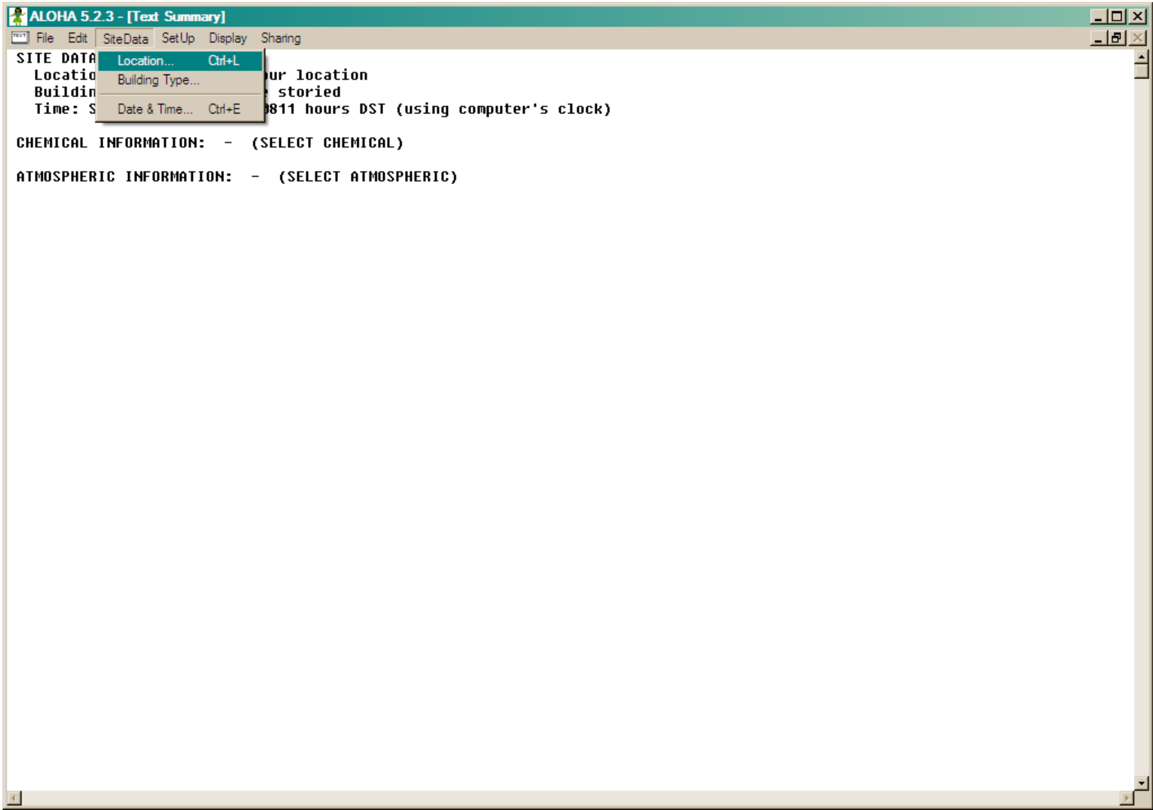
Analysis: The ALOHA chemical database contains properties for 100 wt% nitric acid since only pure chemicals, and not solutions, are part of the ALOHA package. New chemicals can be added to the database. As indicated in the body of the report, a dilute acid solution can be added as a new chemical if sufficient property information is available. For evaporation calculations from chemical pools, the vapor pressure is generally the controlling parameter. The table below shows the sensitivity of HNO_3 vapor pressure to the HNO_3 wt% at 30 °C (Perry, 1997).

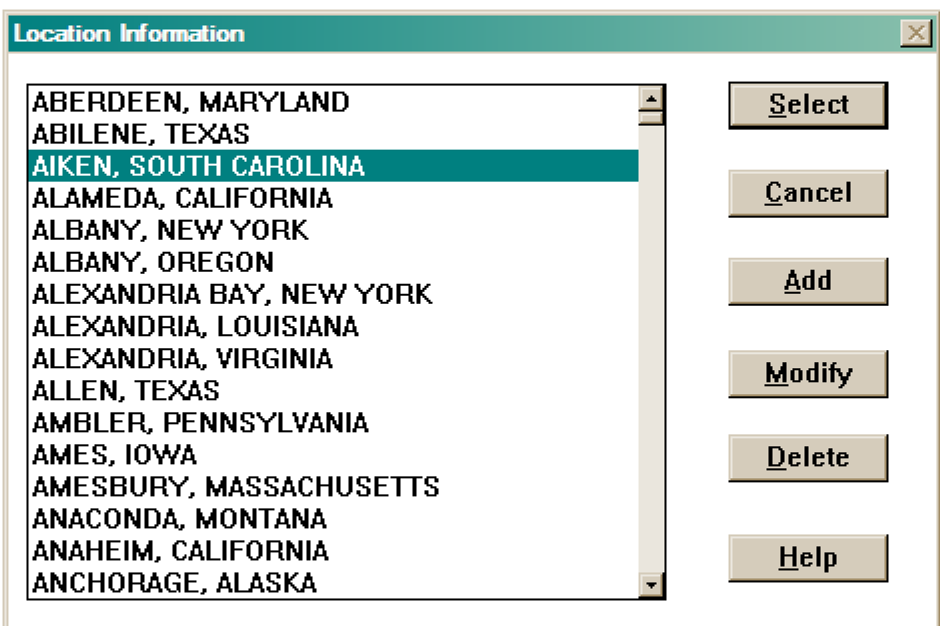
HNO_3 wt%	HNO_3 Vapor Pressure [mm Hg]
40	0.1
50	0.6
60	1.7
70	5.5
80	14
90	36
100	77

In this sample problem, we have assumed concentrated HNO_3 (>90 wt%) and will conservatively analyze the spill on the basis of 100 wt% HNO_3.

Site Data – Location and Building Type

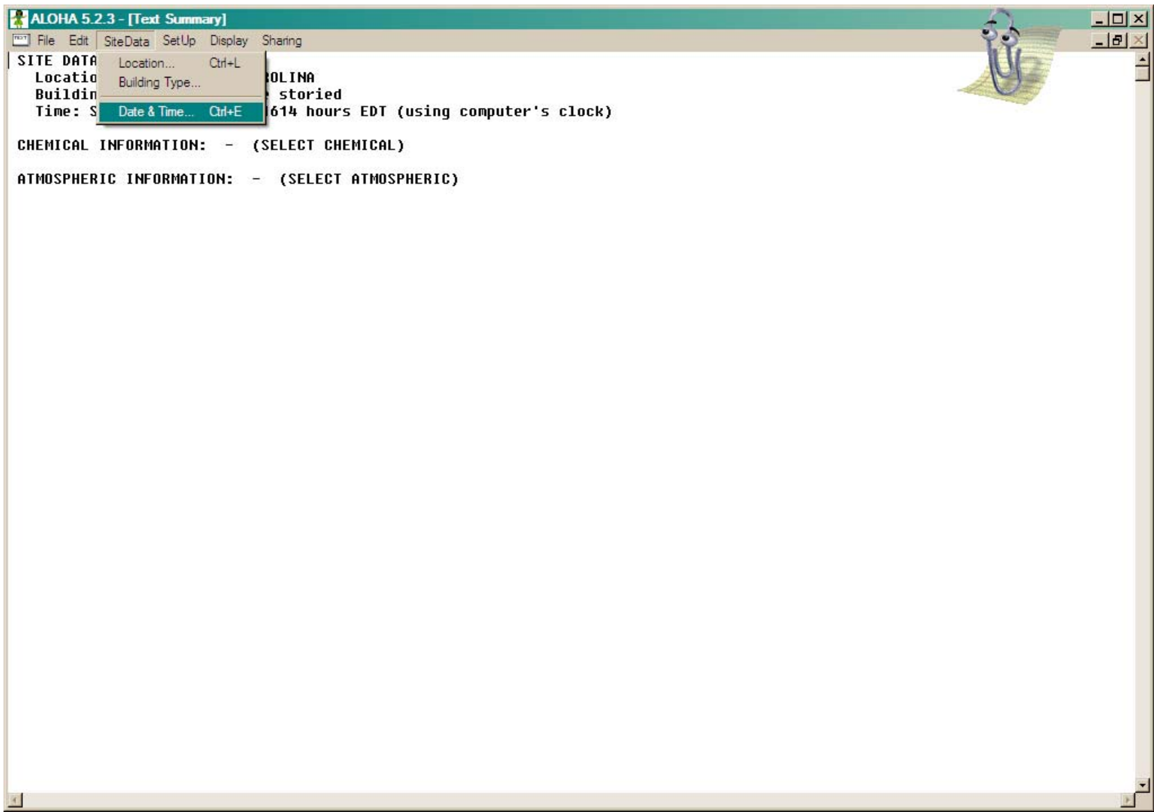
The first step is specifying Aiken, SC as the location. Building Type is not a concern in the analysis since the receptor is assumed to be outdoors consistent with safety analysis practices.

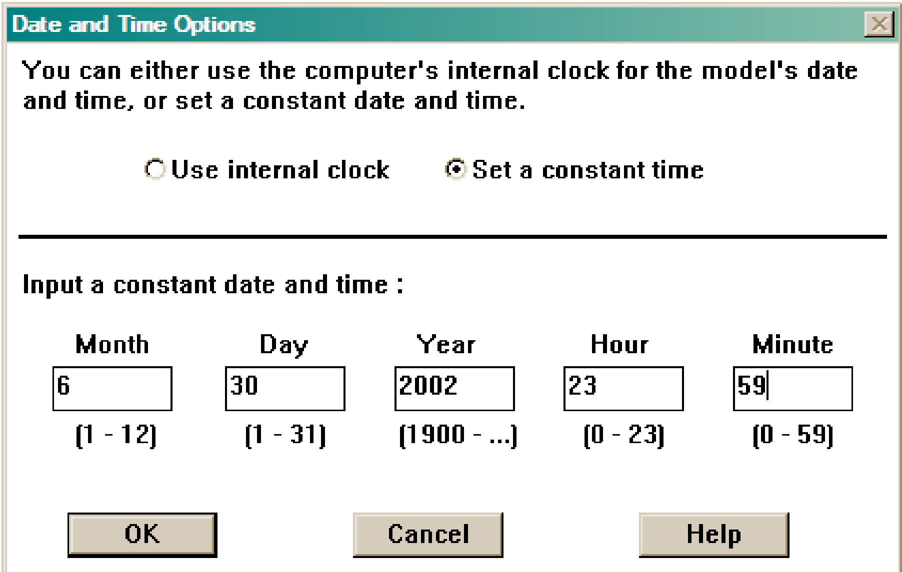

ALOHA 5.2.3 - [Text Summary]
File Edit SiteData SetUp Display Sharing
Location... Ctrl+L
Building Type...
Date & Time... Ctrl+E
SITE DATA
CHEMICAL INFORMATION: - (SELECT CHEMICAL)
ATMOSPHERIC INFORMATION: - (SELECT ATMOSPHERIC)


Location Information
ABERDEEN, MARYLAND
ABILENE, TEXAS
AIKEN, SOUTH CAROLINA
ALAMEDA, CALIFORNIA
ALBANY, NEW YORK
ALBANY, OREGON
ALEXANDRIA BAY, NEW YORK
ALEXANDRIA, LOUISIANA
ALEXANDRIA, VIRGINIA
ALLEN, TEXAS
AMBLER, PENNSYLVANIA
AMES, IOWA
AMESBURY, MASSACHUSETTS
ANACONDA, MONTANA
ANAHEIM, CALIFORNIA
ANCHORAGE, ALASKA
Select
Cancel
Add
Modify
Delete
Help

Site Data - Date and Time

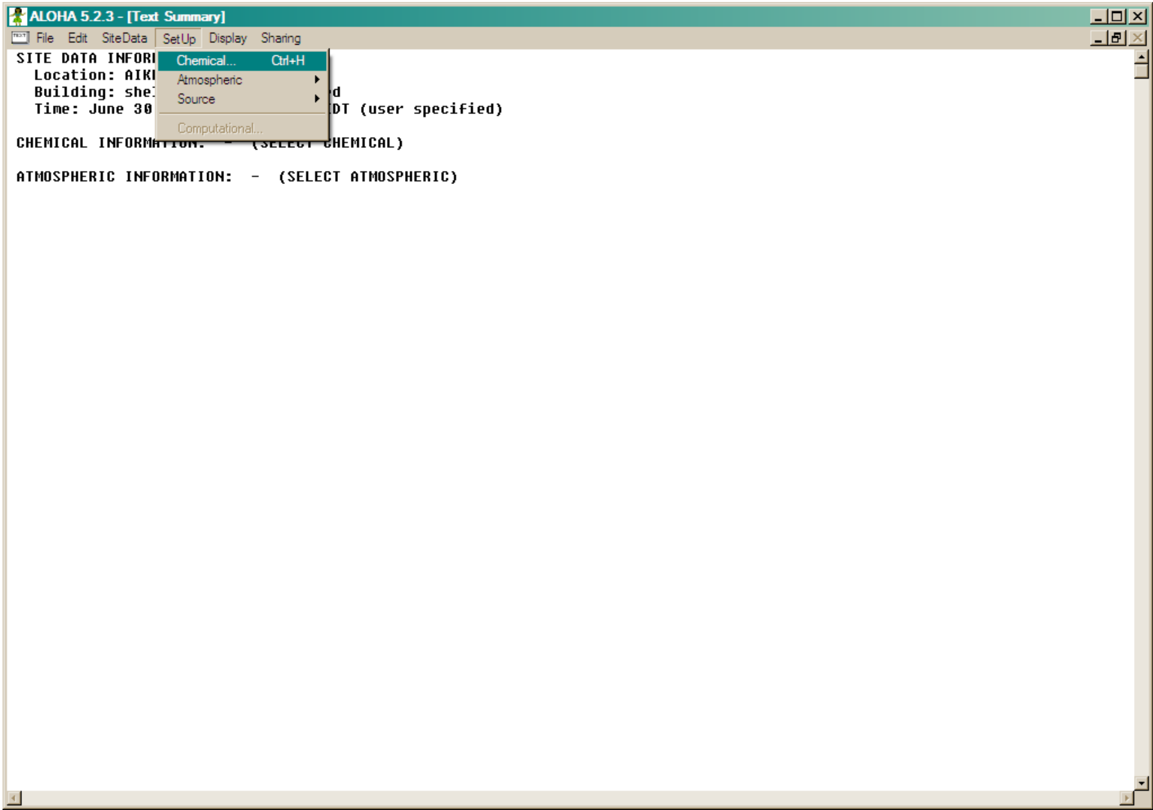
The analysis will be performed for worst-case meteorological conditions. A nighttime release (the time will be set at 23:59) under stable atmospheric conditions will be assumed. For a nighttime release, the date is unimportant (mid-summer day specified following recommendation in the body of the report).

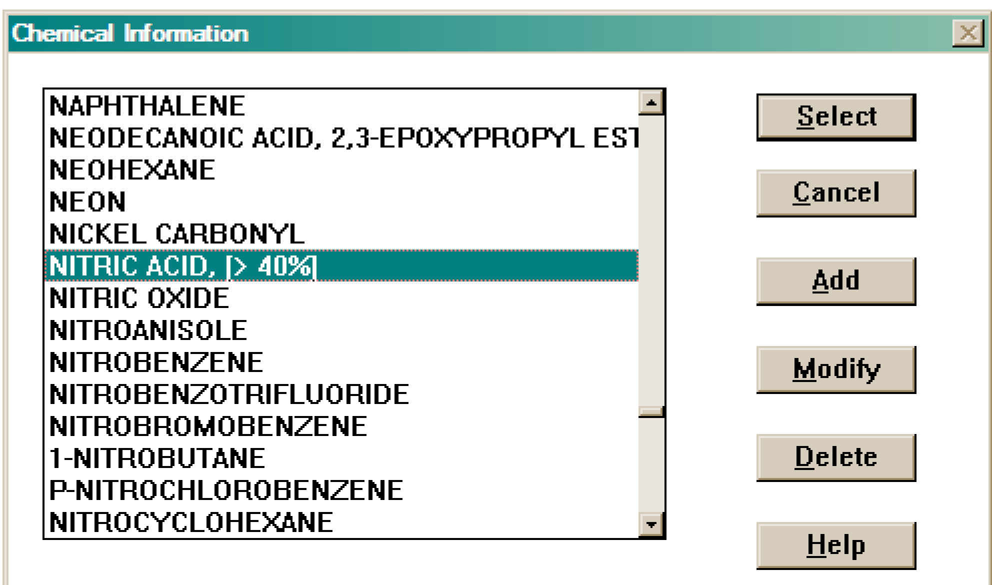




Set Up – Chemical Information

Nitric acid [>40%] is selected from the chemical database. Once nitric acid is selected, chemical properties such as molecular weight, boiling point, and freezing point will appear on the Text Summary screen (shown in screen captures that follow after the chemical information is entered).





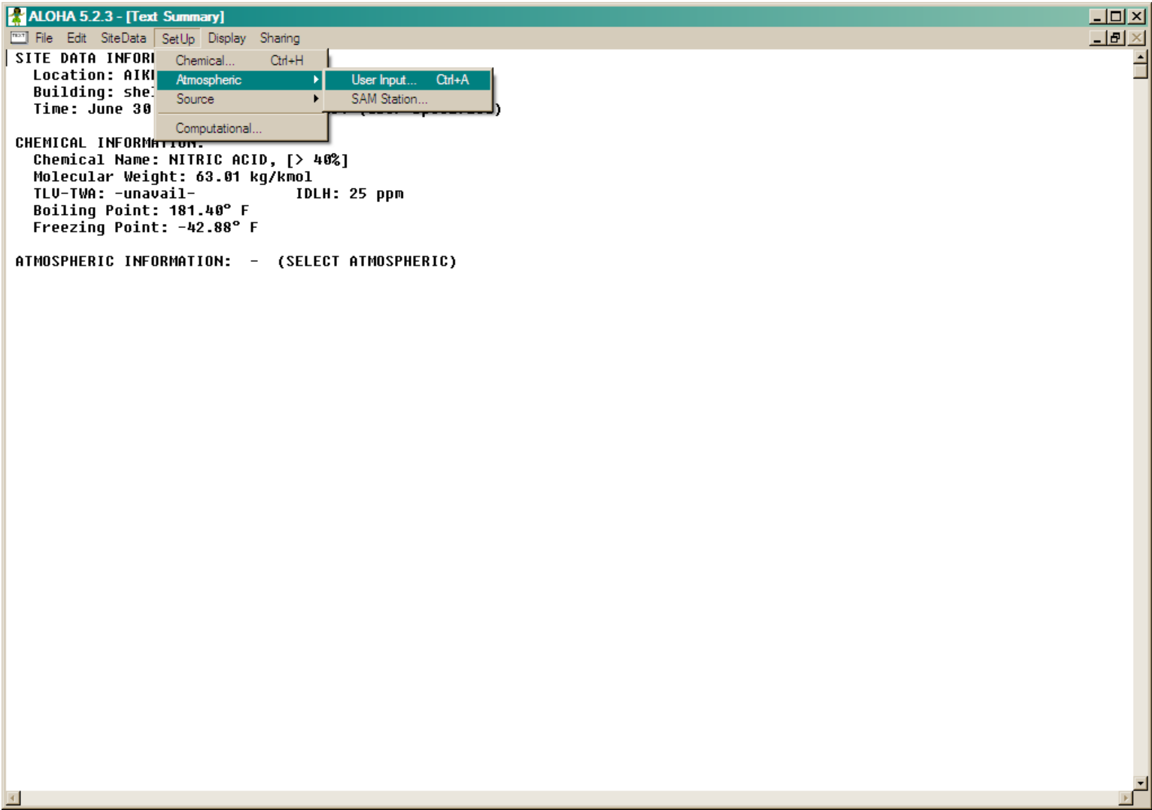
When atmospheric data is entered (e.g. air temperature), other data such as the vapor pressure at ambient temperature will appear. Specifically, ALOHA will determine a vapor pressure of 0.10 atmospheres at 29 °C, which is consistent with the 77 mm Hg cited above for the 100 wt% HNO_3 at 30 °C (Perry, 1997). The ambient saturation concentration is also given, which represents the maximum concentration in air that may be reached by vapor evaporating from a liquid pool (high ambient saturation concentration represents a strong capacity to displace air) (NOAA, 1999a).

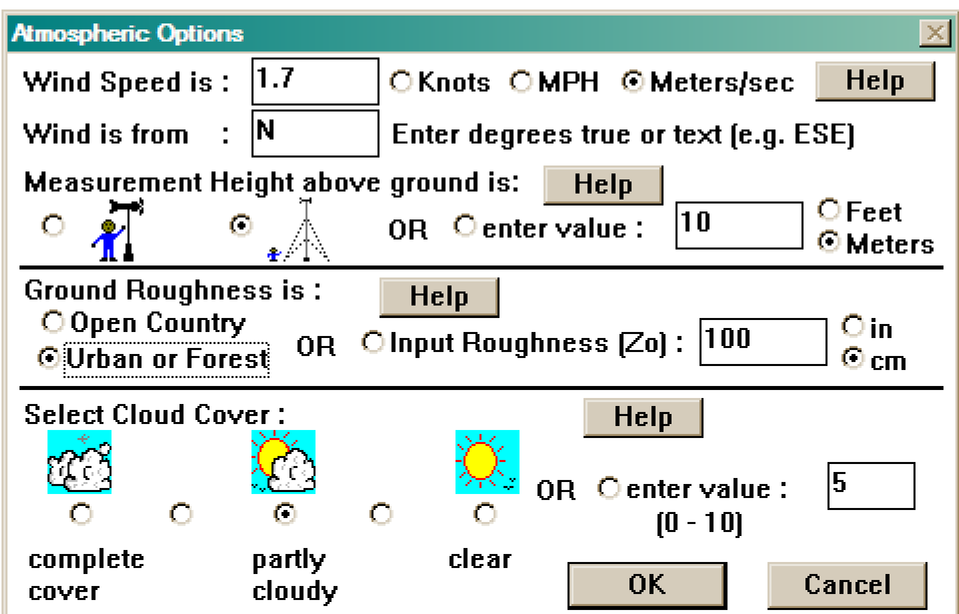
<u>Set Up – Atmospheric Options – User's Input</u>

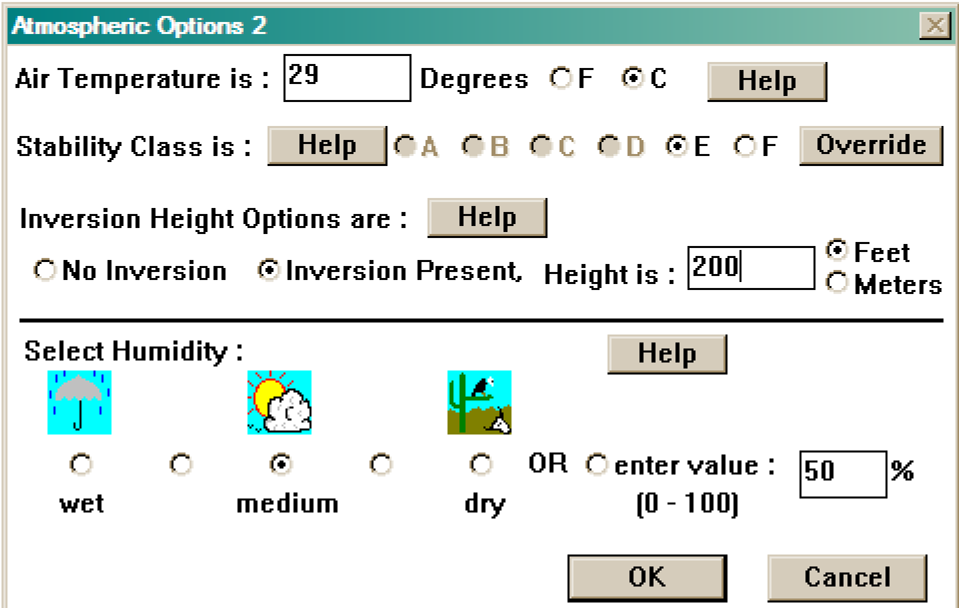
Atmospheric conditions are entered on two dialog boxes that appear on the screen sequentially. On the first screen, wind speed, wind direction, measurement height of wind speed, ground roughness, and cloud cover are entered. On the second screen, air temperature, stability class, inversion height, and humidity are then entered. Since the MW of nitric acid is greater than that of air, the potential exists for dense gas atmospheric transport.

For both neutrally buoyant and dense gas plumes, worst-case meteorological conditions are associated with stable atmosphere and low wind speed. At SRS, the 95th percentile meteorological conditions for both neutrally buoyant and dense gas plumes are taken to be E stability class and 1.7 m/s wind speed (corresponding to measurement height of 10 meter) (Hunter, 1993). The 95th percent highest air temperature is determined from SRS data to be 29 °C (Hunter, 1993). An inversion height of 200 m is taken as worst-case (Holzworth, 1972). At SRS, surface roughness is assumed to be 100 cm, which combines the urban attributes of the operational area with the forested features of the site.

The calculated results are independent of wind direction, so any direction can be specified. Also for a nighttime (or early morning) release, which is consistent with the E stability class, the results will be independent of the amount of cloud cover. Humidity is specified at 50% as discussed in the body report (results are expected to be insensitive to humidity).


ALOHA 5.2.3 - [Text Summary]
File Edit SiteData SetUp Display Sharing
Chemical... Ctrl+H
Atmospheric
Source
Computational...
User Input... Ctrl+A
SAM Station...
SITE DATA INFOR
Location: AIK
Building: she
Time: June 30
CHEMICAL INFORMATION:
Chemical Name: NITRIC ACID, [> 40%]
Molecular Weight: 63.01 kg/kmol
TLV-TWA: -unavail- IDLH: 25 ppm
Boiling Point: 181.40° F
Freezing Point: -42.88° F
ATMOSPHERIC INFORMATION: - (SELECT ATMOSPHERIC)


Atmospheric Options
Wind Speed is :
1.7
Knots
MPH
Meters/sec
Help
Wind is from :
N
Enter degrees true or text (e.g. ESE)
Measurement Height above ground is:
Help
OR
enter value :
10
Feet
Meters
Ground Roughness is :
Help
Open Country
Urban or Forest
OR
Input Roughness (Zo) :
100
in
cm
Select Cloud Cover :
Help
OR
enter value :
5
(0 - 10)
complete cover
partly cloudy
clear
OK
Cancel



Note that based on location, time, wind speed, and cloud cover entries, ALOHA identifies stability classes E and F as compatible (selection bubbles of other stability classes are filled gray).

Set Up – Source – Puddle

The catastrophic rupture of the vessel and subsequent spill of 210 gallons of concentrated HNO_3 is conservatively assumed to spill to the ground and spread unconfined to produce a circular puddle of 1-cm depth. The puddle source configuration is used to model this scenario. The puddle source data are entered on two dialog boxes that appear on the screen sequentially. The user characterizes the spill size in the first dialog box. The user then specifies ground boundary conditions as well as the initial puddle temperature in the second dialog box.

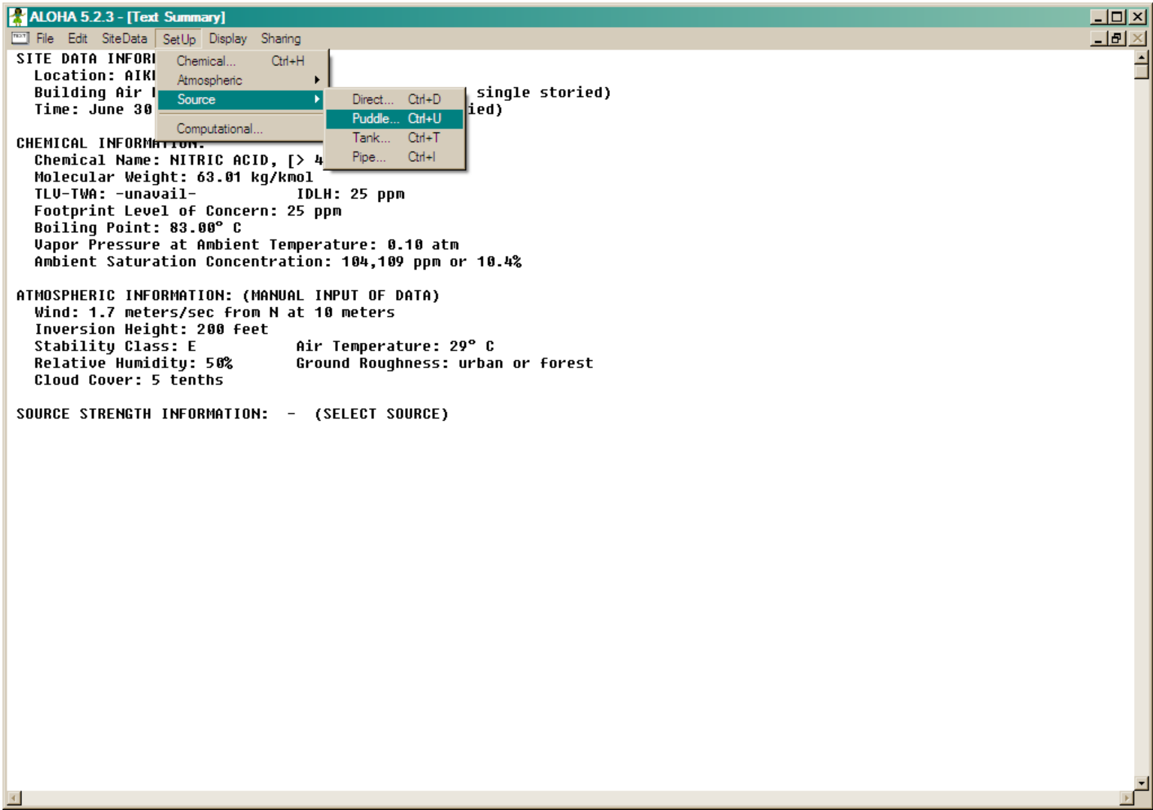
The analyst must first perform a preliminary calculation to determine the puddle diameter (d) or area (A) that is consistent with the 210-gallon volume (V) and 1-cm depth (Δh) specifications.

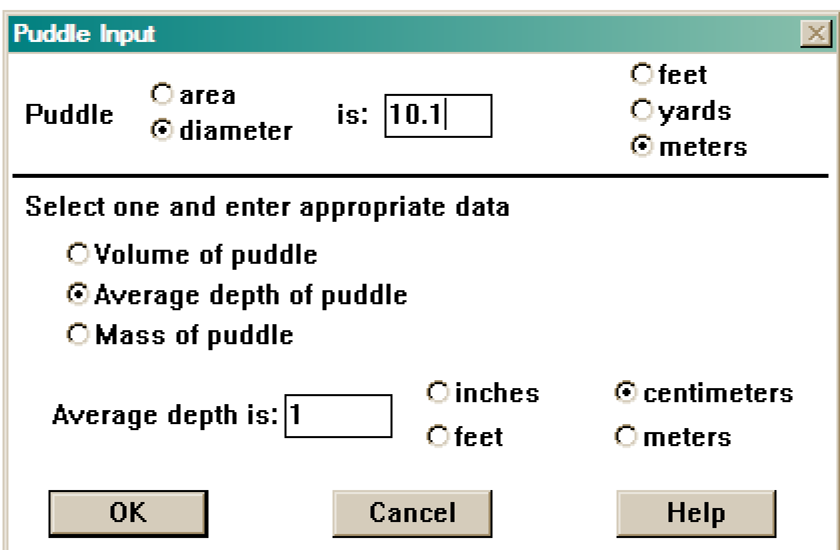
$$A\ [m^2] = V\ [m^3] / \Delta h\ [m] = (210\ [gal] \times 0.003785\ [m3/gal]) / (1\ [cm] \times 0.01\ [m/cm]$$

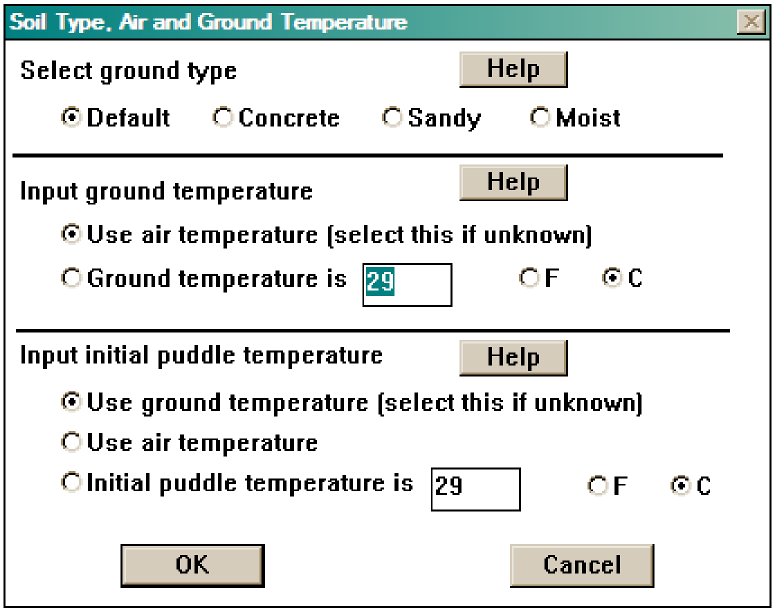
$$A\ [m^2] = 79.5\ m^2$$

$$d\ [m] = (4/\pi \times A\ [m^2])^{0.5} = (4/\pi \times 79.5\ [m^2])^{0.5} = 10.1\ m$$

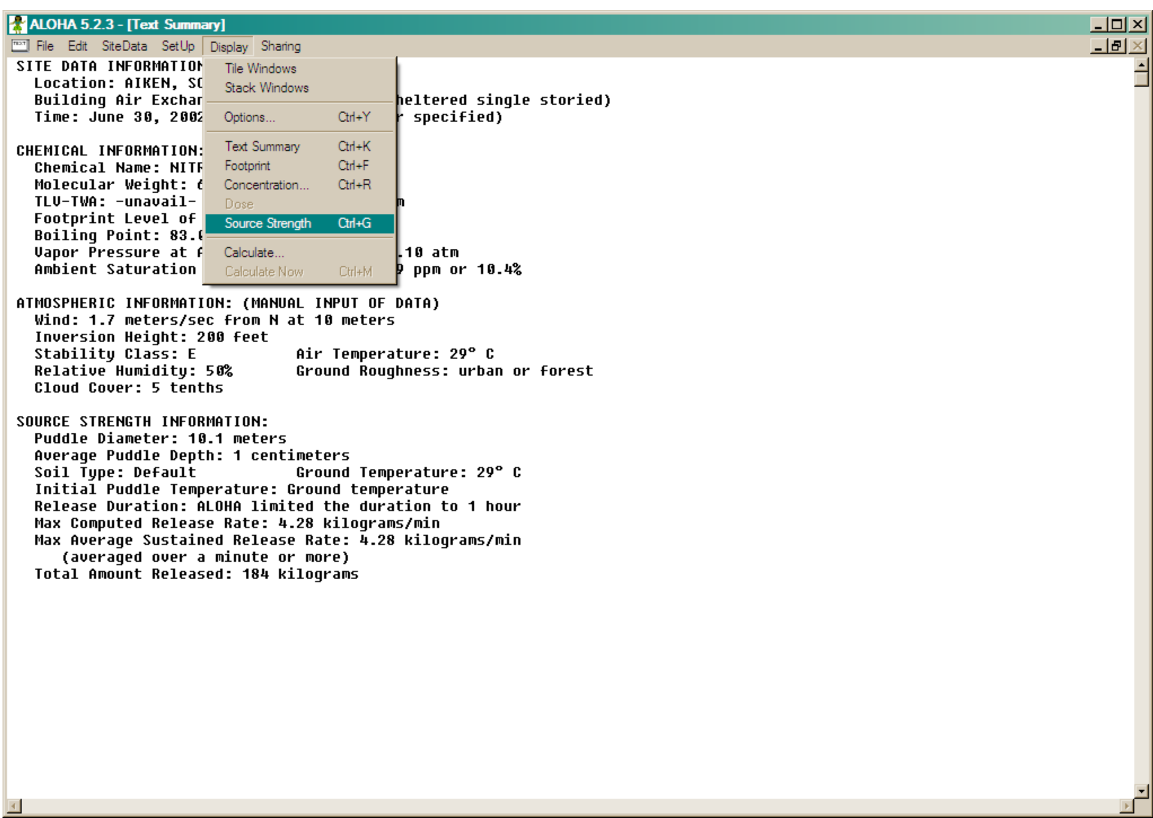
Since the problem statement does not specify a ground type, the default ground type is selected since it is expected to support the calculation of reasonably conservative evaporation rates. No information is available on the ground temperature, so the ground temperature is set equal to the air temperature (default specification). Since the problem statement indicates the HNO_3 is stored at ambient conditions and the ground temperature is assumed to be equal to the air temperature, the initial temperature of the puddle is set equal to the ground and air temperature of 29 °C.



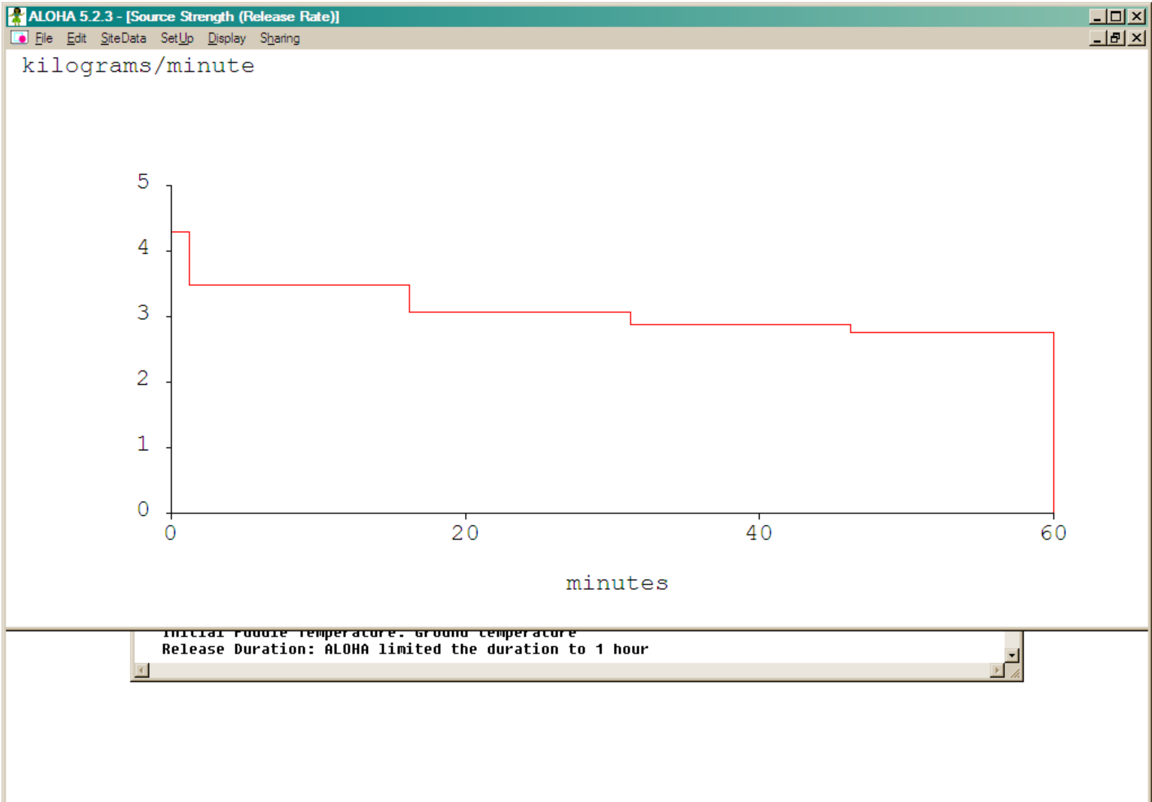




Following data entry above, the Text Summary screen now displays the maximum computed evaporation rate of 4.28 kilograms per minute. The maximum average sustained evaporation rate (over a minute or more) is also determined to be 4.28 kilograms per minute. ALOHA also determines the release to last more than one hour and that 184 kilograms are released in the first hour. The Text Summary screens that follow will display this information.

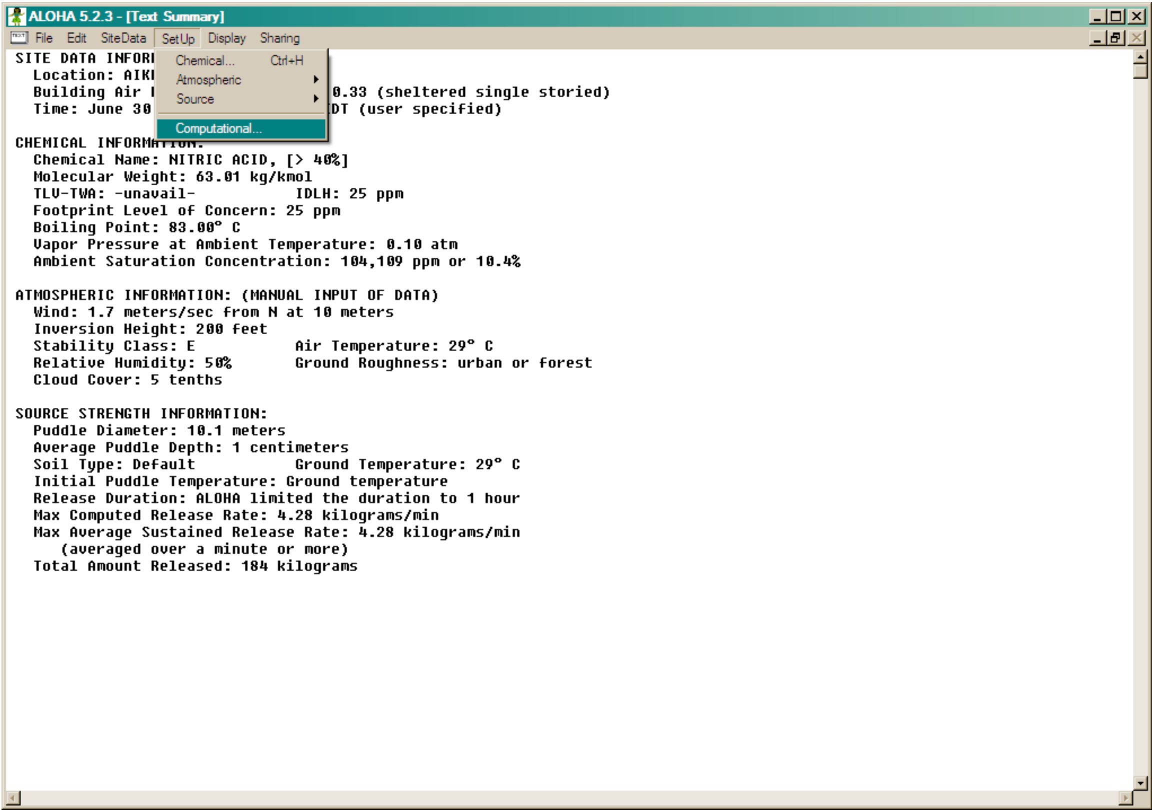


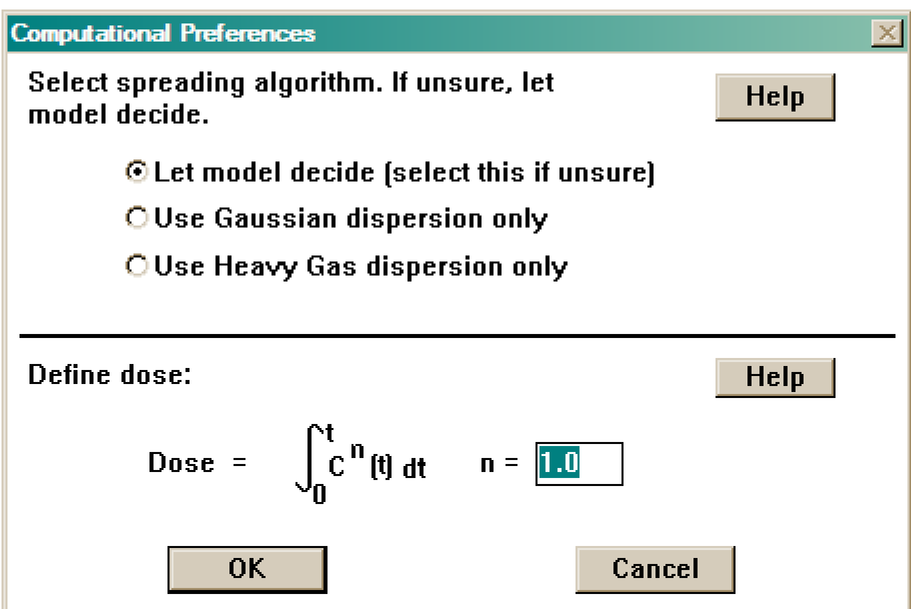
At this point, a graphical representation of the source strength (i.e., evaporation rate) as a function of time can be viewed. Note that the five averaging periods are clearly evident by the stair-step nature of the curve.



Set Up – Computational

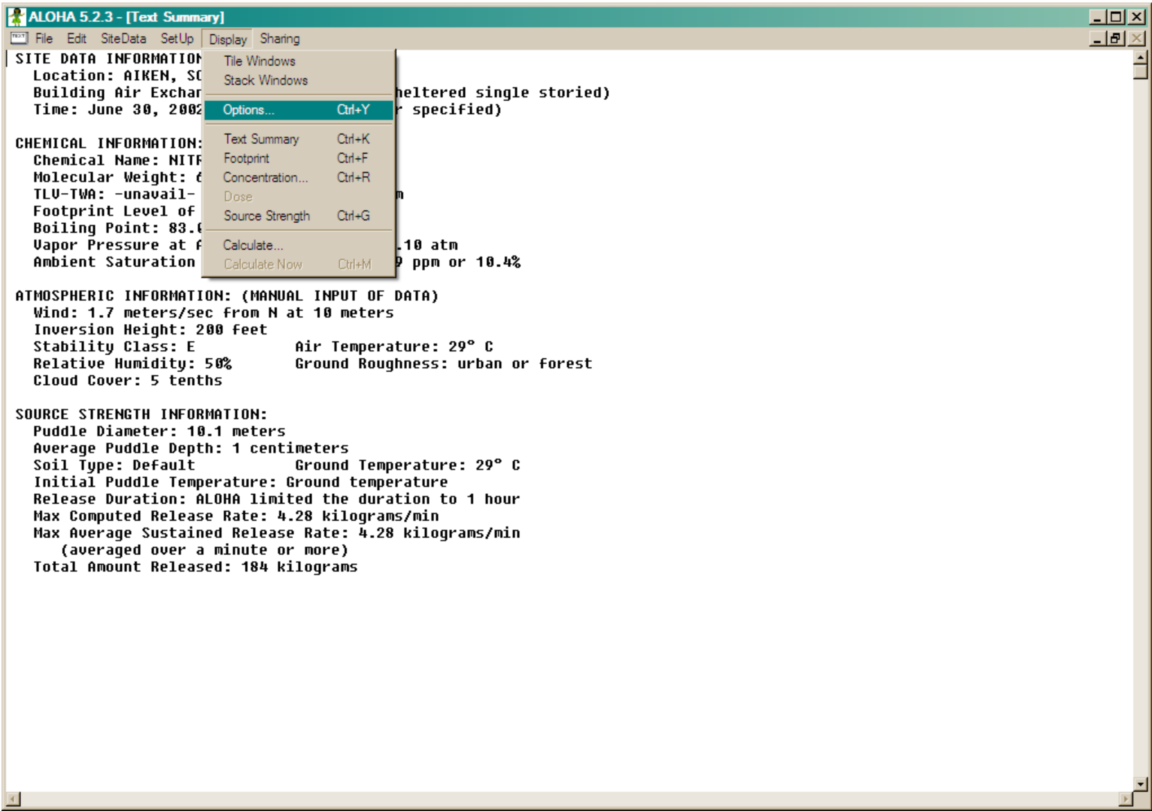
Here, the analyst indicates the recommended preference of letting ALOHA consider both heavy-gas and Gaussian dispersion models and to determine the appropriate model based on the source Ri number. Also under this submenu is the dose exponent input, which is not used in safety analysis since human health evaluation guidelines, such as ERPGs and TEELs, are based on concentration limits and not dose limits.

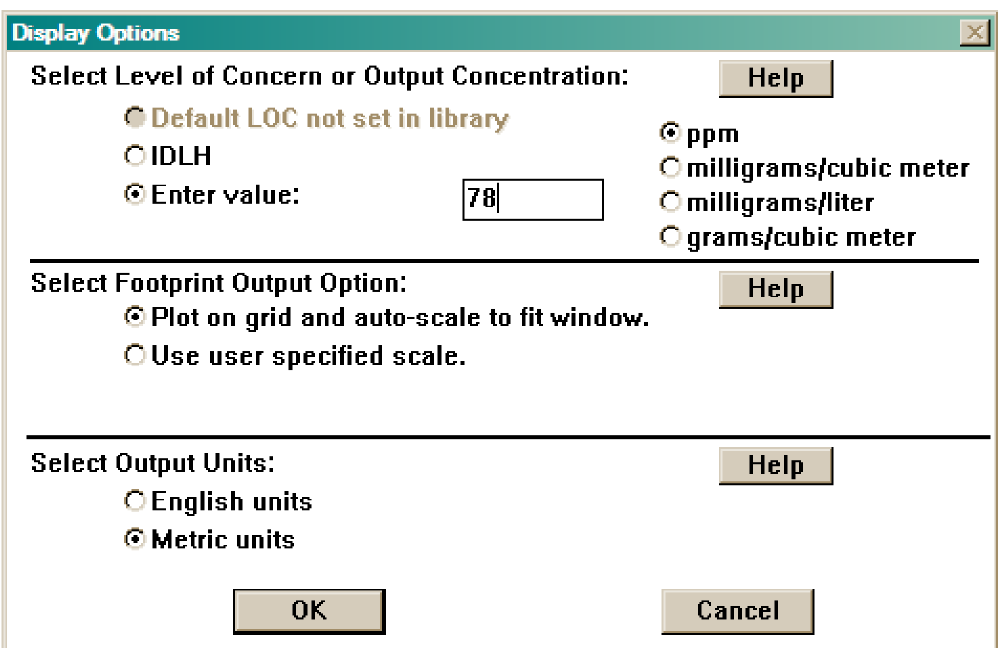




Display – Options

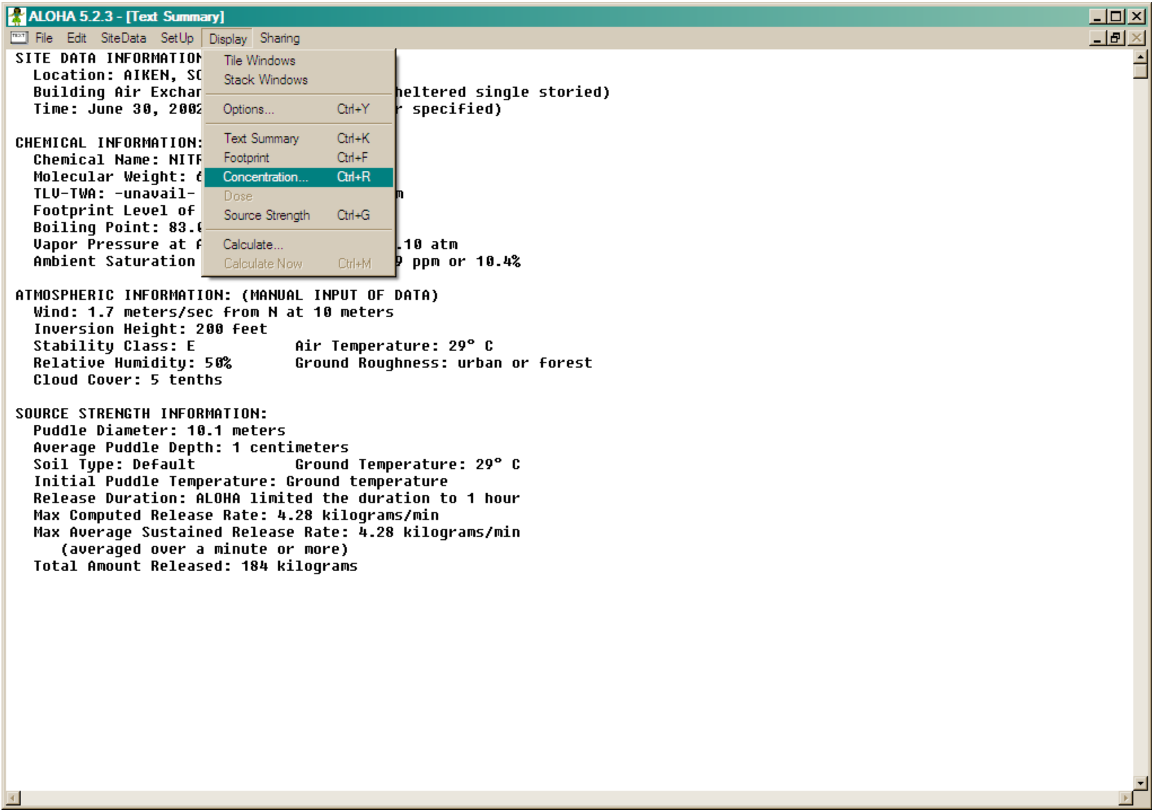
The ERPG-3 value of 78 ppm is entered as the LOC value.

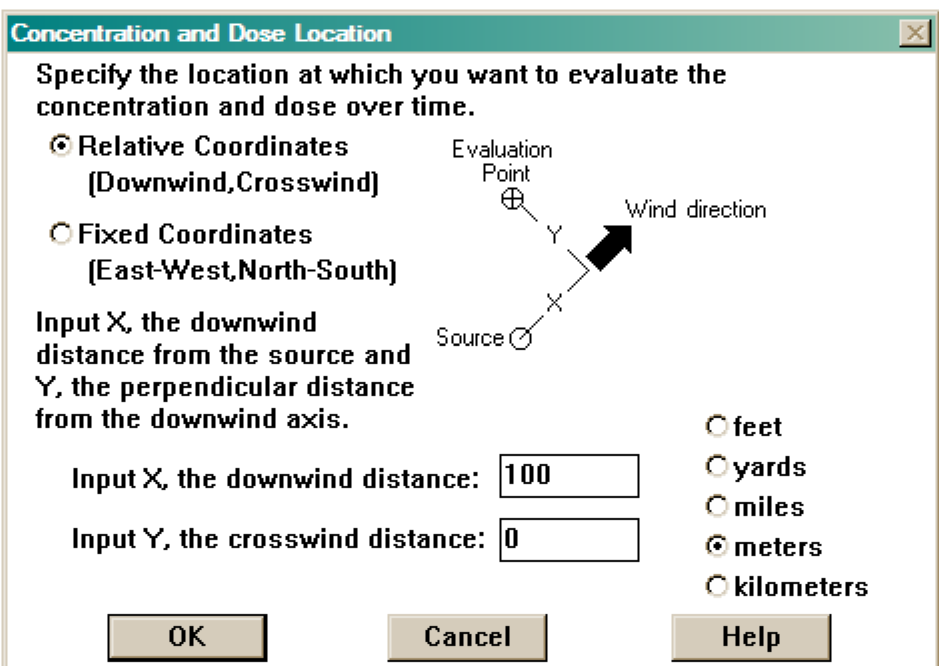


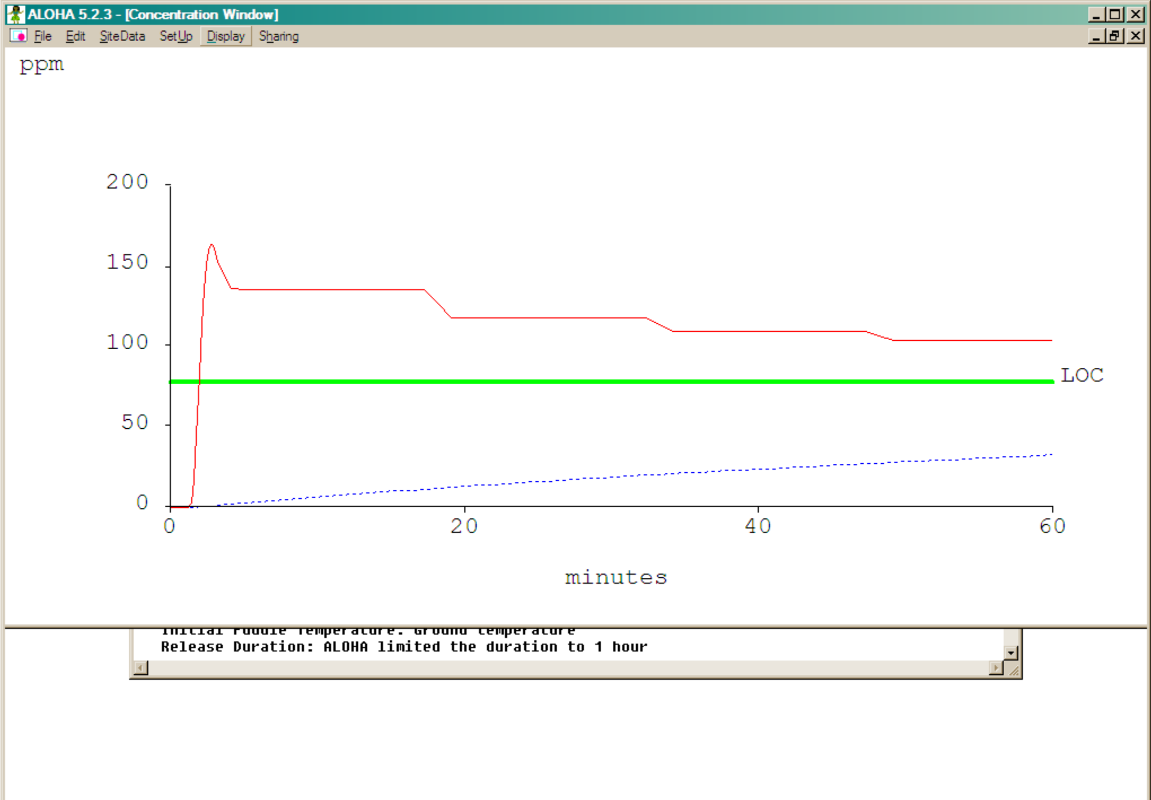


Display – Concentration

The concentration on the centerline (y =0) at 100 can now be determined and compared with ERPG-3 value of 78 ppm.



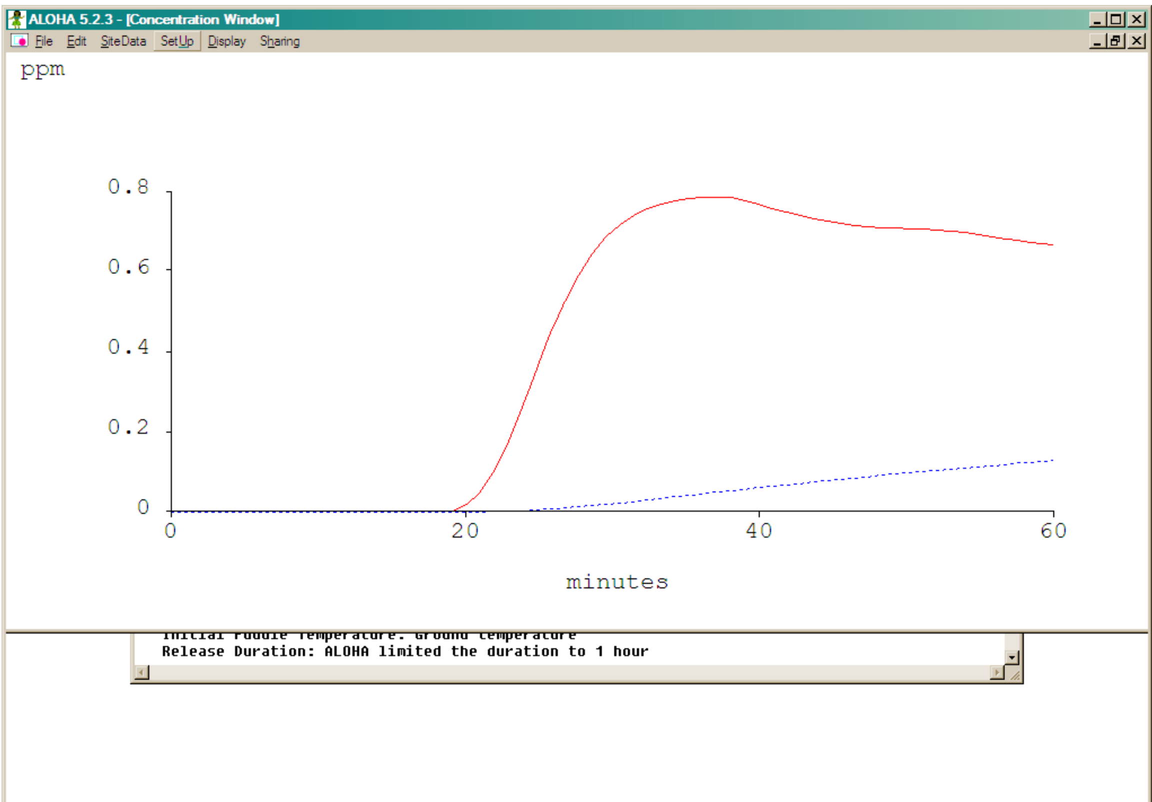





```
SITE DATA INFORMATION:
  Location: AIKEN, SOUTH CAROLINA
  Building Air Exchanges Per Hour: 0.33 (sheltered single storied)
  Time: June 30, 2002  2359 hours EDT (user specified)

CHEMICAL INFORMATION:
  Chemical Name: NITRIC ACID, [> 40%]
  Molecular Weight: 63.01 kg/kmol
  TLV-TWA: -unavail-            IDLH: 25 ppm
  Footprint Level of Concern: 78 ppm
  Boiling Point: 83.00° C
  Vapor Pressure at Ambient Temperature: 0.10 atm
  Ambient Saturation Concentration: 104,109 ppm or 10.4%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)
  Wind: 1.7 meters/sec from N at 10 meters
  Inversion Height: 200 feet
  Stability Class: E            Air Temperature: 29° C
  Relative Humidity: 50%        Ground Roughness: urban or forest
  Cloud Cover: 5 tenths

SOURCE STRENGTH INFORMATION:
  Puddle Diameter: 10.1 meters
  Average Puddle Depth: 1 centimeters
  Soil Type: Default            Ground Temperature: 29° C
  Initial Puddle Temperature: Ground temperature
  Release Duration: ALOHA limited the duration to 1 hour
  Max Computed Release Rate: 4.28 kilograms/min
  Max Average Sustained Release Rate: 4.28 kilograms/min
     (averaged over a minute or more)
  Total Amount Released: 184 kilograms

FOOTPRINT INFORMATION:
  Model Run: Heavy Gas
  User-specified LOC: 78 ppm
  Max Threat Zone for LOC: 153 meters

TIME DEPENDENT INFORMATION:
  Concentration Estimates at the point:
  Downwind:       100 meters
  Off Centerline: 0 meters
  Max Concentration:
     Outdoor: 163 ppm
```

One can see from the concentration graph that it takes a few minutes for the plume to reach the receptor at 100 meters. Once the plume reaches the receptor, the receptor is exposed to concentrations in excess of 78 ppm. From the Text Summary screen, the maximum concentration is given as 163 ppm. The Text Summary screen also indicates that ALOHA used the heavy gas dispersion algorithm to calculation the downwind concentration.

The second case of the problem statement involves calculating the maximum concentration at 2500 meters downwind and comparing it with the ERPG-2 value of 6 ppm. The details of changing the input data for this case are not shown since they involve steps similar to those already shown. The concentration graph and Text Summary screen for this second case are shown below.



```
ALOHA 5.2.3 - [Text Summary]
File  Edit  SiteData  SetUp  Display  Sharing
SITE DATA INFORMATION:
   Location: AIKEN, SOUTH CAROLINA
   Building Air Exchanges Per Hour: 0.33 (sheltered single storied)
   Time: June 30, 2002  2359 hours EDT (user specified)

CHEMICAL INFORMATION:
   Chemical Name: NITRIC ACID, [> 40%]
   Molecular Weight: 63.01 kg/kmol
   TLV-TWA: -unavail-            IDLH: 25 ppm
   Footprint Level of Concern: 6 ppm
   Boiling Point: 83.00° C
   Vapor Pressure at Ambient Temperature: 0.10 atm
   Ambient Saturation Concentration: 104,109 ppm or 10.4%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)
   Wind: 1.7 meters/sec from N at 10 meters
   Inversion Height: 200 feet
   Stability Class: E            Air Temperature: 29° C
   Relative Humidity: 50%        Ground Roughness: urban or forest
   Cloud Cover: 5 tenths

SOURCE STRENGTH INFORMATION:
   Puddle Diameter: 10.1 meters
   Average Puddle Depth: 1 centimeters
   Soil Type: Default            Ground Temperature: 29° C
   Initial Puddle Temperature: Ground temperature
   Release Duration: ALOHA limited the duration to 1 hour
   Max Computed Release Rate: 4.28 kilograms/min
   Max Average Sustained Release Rate: 4.28 kilograms/min
      (averaged over a minute or more)
   Total Amount Released: 184 kilograms

FOOTPRINT INFORMATION:
   Model Run: Heavy Gas
   User-specified LOC: 6 ppm
   Max Threat Zone for LOC: 800 meters

TIME DEPENDENT INFORMATION:
   Concentration Estimates at the point:
   Downwind:        2500 meters
   Off Centerline: 0 meters
   Max Concentration:
      Outdoor: 0.783 ppm
```

One can see from the concentration graph that it takes approximately 20 minutes for the plume to reach the receptor at 2500 meters. The receptor at 2500 meters is not exposed to the maximum plume concentration until almost 20 minutes later. From the Text Summary screen, the maximum concentration is given as 0.78 ppm.

The Text Summary screen also indicates that ALOHA used the heavy gas dispersion algorithm to calculation the downwind concentration. Sensitivity runs (not shown) were performed in which the wind speed was increased from the 1.7 m/s value. At 2.2 m/s wind speed, the transition from heavy gas to Gaussian plume dispersion occurred as determined by ALOHA.

Additional Analysis:

The maximum concentration at 100 meters downwind will now be calculated for an evaporative release from a 210-gallon puddle of 70 wt% HNO_3 and compared with the ERPG-3 value of 78 ppm. This additional calculation will highlight the large difference in evaporation rates between pure HNO_3 and 70 wt% HNO_3. The approach that has been developed at SRS for dilute acids that involves entering pseudo property values for the boiling point, freezing point, critical pressure, and critical temperature will be used. (Note that calculations are performed with an earlier version of ALOHA, namely 5.2.2, since the dilute acids were added to the chemical library of ALOHA 5.2.2. The minor differences between version 5.2.2 and version 5.2.3 are not expected to alter the calculations in any significant way.) Recall that these pseudo property values are set through trial and error so that the ALOHA chemical database calculates vapor pressures at the temperature range of interest that closely match the vapor pressures for the dilute acid as found in a reference book. From the table of HNO_3 vapor pressure at 30 °C as a function of weight percent shown earlier, the vapor pressure for HNO_3 70 wt% is 5.5 mm Hg (0.0072 atmospheres) compared to 77 mg Hg (0.10 atmospheres) for pure the HNO_3 (Perry, 1997). Therefore, a much lower evaporation rate and 100-m concentration can be expected since the vapor pressure for 70 wt% HNO_3 is approximately 7% of that for 100 wt% HNO_3. Results are shown below.

```
ALOHA 5.2.2 - [Text Summary]
File  Edit  SiteData  SetUp  Display  Sharing
SITE DATA INFORMATION:
  Location: AIKEN, SOUTH CAROLINA
  Building Air Exchanges Per Hour: 0.33 (Sheltered single storied)
  Time: June 30, 2002  2359 hours EDT (User specified)

CHEMICAL INFORMATION:
  Chemical Name: NITRIC ACID 70%     WSMS
  Molecular Weight: 63.01 kg/kmol
  TLV-TWA: 2 ppm               IDLH: 25 ppm
  Default LOC from Library: 2 ppm
  Footprint Level of Concern: 78 ppm
  Boiling Point: 137.45° C
  Vapor Pressure at Ambient Temperature: 0.0070 atm
  Ambient Saturation Concentration: 7,116 ppm or 0.71%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)
  Wind: 1.7 meters/sec from 0° true at 10 meters
  Inversion Height: 200 feet
  Stability Class: E           Air Temperature: 29° C
  Relative Humidity: 50%       Ground Roughness: Urban or forest
  Cloud Cover: 5 tenths

SOURCE STRENGTH INFORMATION:
  Puddle Diameter: 10.1 meters
  Average Puddle Depth: 1 centimeters
  Soil Type: Default           Ground Temperature: 29° C
  Initial Puddle Temperature: Ground temperature
  Release Duration: ALOHA limited the duration to 1 hour
  Max Computed Release Rate: 278 grams/min
  Max Average Sustained Release Rate: 270 grams/min
     (averaged over a minute or more)
  Total Amount Released: 15.5 kilograms

TIME DEPENDENT INFORMATION:
  Concentration Estimates at the point:
  Downwind:       100 meters
  Off Centerline: 0 meters
  Max Concentration:
     Outdoor: 11.6 ppm
     Indoor:  3.08 ppm
  Note: Indoor graph is shown with a dotted line.
```

Comparison of the 70 wt% HNO_3 results with the pure HNO_3 and results are summarized below.

	70 wt% HNO_3	100 wt% HNO_3
Vapor Pressure [atm]	0.00070	0.01
Vapor Pressure [mm Hg]	0.53	76
Vapor Pressure at 30 °C[mm Hg] (Perry, 1997)	0.55	77
Max. Computed Release Rate [kg/min]	0.278	4.28
Max. Concentration at 100 m [ppm]	11.6	163

Note that the maximum computed release rate and maximum concentration at 100 meters for the 70 wt% HNO_3 case are approximately 7% of the values calculated for the 100 wt% HNO_3 case, (recall vapor pressure proportional relationship was also 7%).

8.0 ACRONYMS & DEFINITIONS

Selected Terms and Definitions Used in Source Term, Atmospheric Transport and Dispersion, and Consequence Analysis

Advection – The transport of a fluid property by the bulk motion of the fluid, sometimes called convection in engineering terminology.[30]

Aerosol – Solid or liquid particles (droplets) that are suspended in a gas or vapor medium.

Atmospheric Stability Class – Characterization of the state of atmospheric turbulence. The different atmospheric stability classes typically used by meteorologist range from A for very unstable conditions to F (or sometimes G) for very stable conditions and account for differing levels of buoyant turbulence. High levels of buoyant turbulence are associated with unstable conditions.

Atmospheric Transport and Dispersion – The movement and dilution of a contaminant cloud under the influence of the prevailing wind flows and associated atmospheric turbulence.

Buoyant Turbulence – Atmospheric turbulence that is generated by solar heating of the ground and the formation of thermal updrafts.

Cloud – The volume that encompasses a chemical (contaminant) emission.

Dense Gas (Heavy Gas) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that can occur when the density of the chemical cloud at the source is greater than that of the ambient air (i.e., negatively buoyant cloud). In dense-gas atmospheric transport and dispersion, the dense-gas cloud resists the influences of the hydraulic pressure field associated with the atmospheric wind, and the cloud alters the atmospheric wind field in its vicinity. Dense-gas releases undergo what has been described in the literature as "gravitational slumping". Gravitational slumping is characterized by significantly greater lateral (crosswind) spreading and reduced vertical spreading as compared to the spreading that occurs with a neutrally buoyant release.

Dilution – The reduction of the cloud concentration due to mixing with ambient air.

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[30] Some of the definitions for atmospheric transport and dispersion terms are taken from the Chemical Dispersion and Consequence Assessment Working Group of the DOE-sponsored Accident Phenomenology and Consequence Methodology Evaluation Program (Lazaro, 1997).

Dispersion – Spreading of the cloud boundaries due to atmospheric turbulence. Atmospheric, turbulent dispersion is the result of rapid and irregular fluctuations in wind components, such as velocity.

Dispersion Coefficients – A measure of the spreading of a contaminant cloud as it travels downwind. In Gaussian puff and plume formulations:

σ_x = longitudinal dispersion coefficient (function of downwind distance, x), representing the standard deviation of the concentration distribution in the downwind axis direction;

σ_y = horizontal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the crosswind axis direction; and

σ_z = vertical dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the vertical axis direction.

Emergency Response Planning Guidelines (ERPGs) – Estimates of concentrations for specific chemicals above which acute exposure (up to 1 hour) would be expected to lead to adverse health effects of increasing severity for ERPG-1, ERPG-2, and ERPG-3. The American Industrial Hygiene Association (AIHA) has issued three levels of ERPG values based on toxic effect of the chemical for use in evaluating the effects of accidental chemical releases on the general public (AIHA, 2002). The definitions of each ERPG level in terms of toxic effects are as follows (AIHA, 2002).

ERPG-1*: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing more than mild, transient health effects or without perceiving a clearly defined objectionable odor.*

ERPG-2*: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing irreversible or serious health effects or symptoms that could impair an individual's ability to take protective action.*

ERPG-3*: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.*

Evaporation – Process by which molecules of a liquid come off the surface of a liquid and enter the vapor space.

Flashing – Sudden vaporization of a liquid as a result of the liquid undergoing a sudden change in pressure such that its temperature at the new pressure condition is above the boiling point.

Friction Velocity – A measure of the mechanical turbulence and a direct measure of the frictional forces of the wind in the boundary layer adjacent to the earth's surface. It can be thought of as the representing the consequences of Reynolds stresses, which cause velocity fluctuations to transport momentum.[30]

Gaussian Puff/Plume Model – A diffusion model for vapor or gas chemical releases to the environment in which the lateral and vertical distribution of the chemical concentration follow a normal or Gaussian distribution. Additionally in the puff model, the longitudinal distribution follows a normal or Gaussian distribution. A segmented Gaussian puff/plume model incorporates a computational approach in which the Gaussian puff/plume is spatially segmented into individual volume sources with each segment generating a concentration field.[30]

Inversion Layer – A region of air in which the temperature increases with increasing distance from the ground.[30] The stable temperature gradient in the inversion layer suppresses vertical turbulence and mixing. In addition, the inversion layer acts as a cap to rising thermals of air from below. Thus, the inversion layer restricts the range and magnitude of vertical turbulence. The vertical extent of this elevated inversion is known as the inversion layer height (z_i). The region below z_i is often referred to as the mixed or mixing layer. In Gaussian dispersion modeling, the inversion layer is generally assumed to act as barrier that contains the contaminant cloud below z_i.

Level of Concern (LOC) – Term used by ALOHA to refer to a concentration limit that is used for consequence assessment (e.g., assessment of human health risks from contaminant plume exposure). Safety analysis work uses the emergency response planning guidelines (ERPGs) and temporary emergency exposure limits (TEELs) for assessing human health effects for both facility workers and the general public.

Liquefied Gas – A chemical substance that is a vapor at atmospheric pressure and temperature, but is stored as a liquid. The chemical substance in storage may be either cooled (i.e., refrigerated) at ambient pressure or pressurized (i.e., compressed) at ambient temperature to achieve and maintain the liquid state. Compressed liquefied gases may be subject to flashing as it discharges from its storage vessel.

Mechanical Turbulence – Atmospheric turbulence that is generated from the shear forces that result when adjacent parcels of air move at different velocities (i.e. either at different speeds or directions). Fixed objects on the ground such as buildings or trees increase the ground roughness and increase mechanical turbulence in proportion to their size.

Neutrally Buoyant (Passive) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that occurs when the density difference between the chemical cloud and the ambient air is small. A neutrally buoyant cloud does not alter the atmospheric wind field. The term passive is used to describe the phenomenological characteristics associated with atmospheric transport and dispersion of the cloud as the cloud follows the bulk movements and behavior of the atmospheric wind flow.

Permissible Exposure Limit - Time-Weighted Average (PEL-TWA) – Chemical concentration limits that are developed by the Occupational Safety & Health Administration for use in limiting worker exposures to airborne chemicals.

Plume – Term used to describe the form of the chemical cloud for a sustained or continuous release.

Plume Meander – Variation of the location of the plume centerline (i.e., plume swings back and forth), due to turbulent velocity fluctuations. The receptor on the time-averaged centerline location is only exposed intermittently to the concentration of the instantaneous plume centerline. As a result, the time-averaged concentration decreases on the centerline and increases on the outer edges of the plume. The magnitude of the plume meander effect on the time-averaged centerline concentration is a function of averaging time.

Positively Buoyant (Passive) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that can occur when the density of the chemical cloud at the source is significantly less than that of the ambient air. A positively buoyant cloud behaves like a neutrally buoyant cloud with the added effect that the positive buoyancy produces upward forces that cause the puff or plume to rise.

Puff – Term used to describe the form of the chemical cloud for an instantaneous release or release of short duration.

Richardson (Ri) Number – Relative measure of the potential energy of the cloud with respect to the mechanical turbulence energy of the atmosphere. Potential energy is associated with buoyancy forces that tend to suppress turbulence. Wind shear generates mechanical turbulence energy.

Source Term – The rate of release (may be time dependent), duration, and physical and energetic characteristics of hazardous material released to the environment. ALOHA uses the term source strength to refer to the time-dependent rate of vapor release to the environment.

Surface Roughness Length (z_o) – Measure of the amount of atmospheric mechanical turbulence that is induced by the presence of surface roughness elements such as vegetation and man-made structures.

Temporary Emergency Exposure Limits (TEELs) – Surrogate ERPG values for chemicals for which ERPGs have not been published (i.e., the TEEL-1, -2, and -3 values) and surrogate Permissible Exposure Limit - Time-Weighted Average (PEL-TWA) values for all chemicals for which PEL-TWA values have been published (i.e., TEEL-0 values).

Vapor – The gas produced from the evaporation of a liquid.

Vapor Pressure – The equilibrium pressure of the pure component vapor over the pure component liquid. When a chemical exists in a solution or mixture, the term partial pressure is generally used.

95th Percentile Meteorology/Consequence – A method described in the U.S. Nuclear Regulatory Commission Regulatory Guide 1.145 (February 1983) to define the meteorological conditions assumed to be present for consequence analysis. Given site-specific data, the 95th percentile meteorology is the set of meteorological conditions assumed during a postulated release to a downwind receptor location that would result in a dose that is exceeded 5% of the time (based on a yearly average). This consequence level is direction-independent, i.e. averaged over all 360^{o} at the distance of interest.

9.0 REFERENCES

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APPENDIX A: ATMOSPHERIC TRANSPORT AND DISPERSION MODELS

The ALOHA code considers two classes of atmospheric transport and dispersion based upon the released chemical cloud density and how it affects the interaction of the chemical cloud with the atmospheric wind flow. For airborne releases in which the initial chemical cloud density is less than or equal to that of the ambient air, ALOHA treats the released chemical as being neutrally buoyant and as undergoing passive atmospheric transport and dispersion. If the density of the initial chemical cloud is greater than that of the ambient air, then the possibility exists for either passive or dense-gas type of atmospheric transport and dispersion. Dense gas behavior at the source is determined on the basis of the source Ri number having a value greater than one.[31]

The algorithms for both neutrally buoyant and dense-gas atmospheric transport and dispersion compute time-dependent, ground-level concentrations at a singular downwind location. In addition, ALOHA will generate a footprint plot that shows the area (in terms of longitudinal and lateral boundaries) where the ground-level concentration reached or exceeded the LOC during puff or plume passage.

ALOHA allows for meteorological data from a portable weather station to be captured and used in the atmospheric transport and dispersion calculations or for the user to manually input values for meteorological parameters that remain constant during the scenario duration. The ALOHA documentation refers to a portable weather station as a station for atmospheric measurements (SAM). The SAM samples wind speed and direction every two seconds. This capability is extremely useful for field use in emergency response situations. For safety analysis applications, however, the user analyzes a prescribed, hypothetical scenario and directly inputs the meteorological parameters that are necessary to perform the calculations.

NEUTRALLY BUOYANT MODEL

A neutrally buoyant chemical cloud that is released to the atmosphere does not alter the atmospheric wind flow, and therefore, the term passive is used to describe the phenomenological characteristics associated with its atmospheric transport and dispersion. As a passive contaminant, the released chemical follows the bulk movements and behavior of the atmospheric wind flow.

Technical Background of Gaussian Dispersion Models

Time-averaged concentrations obtained from field studies of neutrally buoyant chemical releases are observed to follow Gaussian or bell-shaped distributions. The Gaussian plume and puff dispersion models that have been developed to predict the outcome of chemical releases that are represented by these field studies are well established and widely used. As the plume develops

[31] Definitions of source Ri number for continuous and instantaneous releases are given by Equations 4-1 and 4-2, respectively.

and moves downwind, it approximates a Gaussian distribution in both the crosswind (lateral) and vertical directions. For continuous releases, the mean wind speed dilutes the chemical concentration but the longitudinal dispersion is negligible. As the plume moves downwind it gets progressively larger due to lateral and vertical dispersion, and hence becomes less concentrated. If the release is of short duration (i.e., puff), the mean wind speed only acts as a transport agent and the turbulence in the longitudinal direction becomes more important. Accordingly, a puff is described by a three-dimension Gaussian equation.

The range of distances over which the Gaussian plume model should be used varies with conditions, but the model is considered generally applicable over the range of 100 m to 10 km and possibly beyond (Hanna, 1982). The basic form for the Gaussian plume model is given below beyond (Hanna, 1982).

$$\chi(x,y,z)=\frac{Q}{2\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \tag{A-1}$$

where:

- χ = atmospheric concentration [mg/m^3] for chemical releases
- Q = source term release rate [mg/s] for chemical releases
- x = downwind distance (relative to source location) [m]
- y = crosswind distance (relative to plume centerline)[m]
- z = vertical axis distance (relative to ground) [m]
- H = effective release height (relative to ground) [m]
- σ_y = horizontal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the crosswind axis direction [m]
- σ_z = vertical dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the vertical axis direction [m]
- u = average wind speed[32] [m/s]

The last term accounts for reflection of the plume at the ground surface through adding an image source at distance H beneath the ground surface.

Note that the concentration is inversely proportional to the wind speed (i.e., greater initial dilution with higher wind speeds).[33] The concentration is also inversely proportional to the

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[32] Since the wind speed varies with distance above the earth's surface, the wind speed value in the Gaussian plume equation will ideally represent some average value over the plume depth, such as the wind speed at the plume centroid (center of mass). In practice, simpler specifications are made such as the wind speed at the effective release height or the wind speed at the height of 10 meters.

horizontal and vertical dispersion coefficients (i.e., higher dispersion enhances the dilution of the puff or plume). These dispersion coefficients are a measure of the effect of atmospheric turbulence in causing the plume to increasingly disperse in the lateral and vertical direction as the plume travels downwind. The dispersion coefficients account for the two sources of atmospheric turbulence, namely, mechanical turbulence and buoyant turbulence.

The horizontal and vertical dispersion coefficients, σ_y and σ_z, required in the Gaussian dispersion equation are obtained either from site-specific meteorological measurements (e.g., standard deviations of wind angles) or through established curves that are based on field experiments and the concept of atmospheric stability class. The averaging time over which the σ_y and σ_z parameters were determined in the field experiments establishes the averaging time for the time-averaged concentrations predicted by the Gaussian dispersion equation. Averaging time is important because greater apparent dispersion occurs with larger averaging time due to plume meander. Plume meander refers to variation of the location of the plume centerline (i.e., plume swings back and forth), due to turbulent velocity fluctuations. The receptor on the time-averaged centerline location is only exposed intermittently to the concentration of the instantaneous plume centerline. As a result, the time-averaged concentration decreases on the centerline and increases on the outer edges of the plume. The magnitude of the plume meander effect on the time-averaged centerline concentration is a function of averaging time.[34] The time-averaging effect on plume meander dispersion is generally accounted for by the following algebraic expression suggested by Gifford that relates the horizontal dispersion coefficient (σ_y) for the averaging time of interest (t_a) to a known reference horizontal dispersion coefficient ($\sigma_{y,ref}$) that is associated with a reference averaging time ($t_{a,ref}$) (Hanna, 1982).

$$\sigma_y = \sigma_{y,ref} \times \left(\frac{t_a}{t_{a,ref}} \right)^q \quad ; \tag{A-2}$$

where, $q = 0.2$ for 3 minutes $< t_a <$ 1 hour

$q = 0.25$ to 0.3 for 1 hour $< t_a <$ 100 hours

Accounting for plume meander effects is typically done for radiological dose analysis, which can be concerned with radiological exposures that are integrated over times that may exceed the reference time for the set of $\sigma_{y,ref}$ values on which the Gaussian dispersion model is based. For

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[33] Calm winds below 0.5 m/s are rare and generally not considered so that evaluating the Gaussian plume equation at a wind speed of zero is not an issue.

[34] In most engineering flow systems, the scales of turbulent motions are limited by the physical size of the system components (e.g., pipe diameter) so that time scales are on the order of seconds or minutes. For these systems, steady statistical averages can be achieved with reasonable sampling periods. Conversely, the range of spatial and time scales in the atmosphere is extremely large. As a consequence, observed statistics are not invariant with averaging time (i.e., one cannot obtain steady mean values since it is not possible to sample atmospheric parameters over a long enough time period) (Wilson, 1995).

chemical consequence analysis, toxic effect on human health can be immediate upon short-duration exposures and the severity of the toxic effect may correlate more closely to concentration than to dose. Thus, an ideal chemical consequence analysis may, in some instances, be concerned with the peak concentrations that may last only a minute or even less. In practice, $\sigma_{y,ref}$ values developed for Gaussian dispersion codes are generally based on averaging times that range from 3 minutes to 1 hour. If the above correlation is be used to calculate (σ_y) for ($t_a < t_{ref}$), a prescribed minimum of t_a equal to 20 seconds has been recommended (Hanna, 1996a).

As the plume travels downwind, its vertical spread may be limited by the presence of an elevated temperature inversion layer. The temperature increases with increasing distance from the ground in the inversion layer. The stable temperature gradient in the inversion layer suppresses vertical turbulence and mixing. In addition, the inversion layer acts as a cap to rising thermals of air from below. Thus, the inversion layer restricts the range and magnitude of vertical turbulence. The vertical extent of this elevated inversion is known as the inversion layer height (z_i). The region below z_i is typically referred to as the mixed or mixing layer. In Gaussian dispersion modeling, the inversion layer is generally assumed to act as barrier that contains the contaminant cloud below z_i. The Gaussian dispersion equation can be modified to consider reflection from the elevated temperature inversion layer.[35] Reflection eventually results in a uniform concentration in the vertical direction (throughout the plume depth from ground to inversion layer boundary).

Determination of σ_y and σ_z from established, empirical curves is a common and acceptable practice. Each σ_y or σ_z curve represents a different atmospheric stability condition based upon the classification scheme first developed by F. Pasquill and later modified by F. A. Gifford. The different atmospheric stability classes range from A for very unstable conditions to F (or sometimes G)[36] for very stable conditions and account for differing levels of buoyant turbulence. High levels of buoyant turbulence are associated with unstable conditions.

The stability class is a function of both the amount of incoming solar radiation and the wind speed. High incoming solar radiation (as would occur on sunny days) and low wind speeds characterize unstable conditions (e.g. stability class A or B) and result in high levels of buoyant turbulence. Under unstable conditions, the air temperature of the atmosphere near the earth's surface declines rapidly with elevation. Warm parcels of air near the surface travel a long

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[35] The ground and the inversion layer boundary are treated as impenetrable and totally reflecting surfaces. Gaussian plume models such as ALOHA treat reflection through addition of mirror image sources both below the ground and above the inversion layer boundary. For reflection off the inversion layer boundary, an addition term is added to Equation (A-1) that is similar to the ground-reflection term with (z-H-$2z_i$) replacing (z+H). Additional terms can be added to account for multiple reflections off the ground and inversion layer boundary. Also at some point downwind (generally where σ_z approaches z_i), the value of the vertical dispersion coefficient, σ_z, in the Gaussian dispersion equation is typically limited to approximately z_i.

[36] ALOHA does not support the input of G stability class.

distance upward before cooling to the temperature of the air around it. As warmer air rises, the cooler air that is displaced sinks downward. Large-scale, convective motions develop that provide substantial vertical mixing. At the other end of the spectrum, stable atmospheric conditions (e.g., stability class E, F or G) can occur on clear nights with low wind speeds. The smaller atmospheric temperature gradient that occurs with stable atmospheric conditions limits upward convection and reduces vertical mixing. Neutral stability conditions (e.g., stability class C or D), tend to occur whenever wind speeds are high or with moderate wind speeds and cloud cover, and represent intermediate stability conditions that produce moderate levels of buoyant turbulence.

Original descriptions and conditions of occurrence given by Pasquill for each stability class are given below (Turner, 1994).

A: Extremely Unstable (Strong superadiabatic). Normally occurs during bright sunshine with relatively low wind speed (< 3 m/s).

B: Moderately Unstable (Moderate superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 3 to 5 m/s range to dim sunshine with wind speeds < 2 m/s.

C: Slightly Unstable (Slight superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 5 to 6 m/s range to dim sunshine with wind speed in the 2 to 3 m/s range.

D: Neutral (Adiabatic). Normally occurs with moderate to dim sunshine, cloudy conditions, and at night, with wind speeds > 3 m/s. It also occurs with very strong wind speeds on either sunny or cloudy days.

E: Slightly Stable (Slight subadiabatic with or without inversion). Normally occurs at night or early morning with some cloud cover and with wind speeds in 2 to 5 m/s range.

F: Moderately Stable (Moderate subadiabatic with inversion). Normally occurs at night or early morning with little cloud cover and with relatively low wind speeds (< 3 m/s).

G: Extremely Stable (Strong subadiabatic with inversion). Normally occurs at night or early morning with very light to nearly zero wind speed.

Different set of dispersion coefficient curves have been established for rural environments and urban environments to account for the additional mechanical turbulence that is generated in urban settings by increased ground roughness due to building structures being taller and spaced closer together. A forest, however, can have a similar effect to that of buildings in increasing ground roughness. A surface roughness length (z_o) is typically used to characterize the amount of mechanical turbulence that is induced by the presence of surface roughness elements. A rule of thumb is that the surface roughness length is approximately one tenth the value of the height of the average surface roughness elements (Hanna, 2002). A surface roughness correction to σ_z

is of the form $(z_o)^r$, where r is in the range of 0.1 to 0.25, with 0.2 being a commonly used value (Hanna, 1982; Hanna, 2002).

Recall that the atmospheric wind speed varies with distance from the ground (z). The wind speed (u) used in the Gaussian plume equation should ideally approximate the wind speed at the plume centroid (center of mass). Typically, the National Weather Service (NWS) measures wind speeds at 10 m (u_{10}). The following formula can be used to estimate the wind speed at other heights (Hanna, 1982).

$$u = u_{10} \times \left(\frac{z}{10}\right)^p \tag{A-3}$$

The power-law exponent parameter (p) can be estimated on the basis of atmospheric stability class and general surface roughness characterization (Hanna, 1982; Irwin, 1979).

Atmospheric Stability Class

	A	B	C	D	E	F
Urban	0.15	0.15	0.20	0.25	0.40	0.60
Rural	0.07	0.07	0.10	0.15	0.35	0.55

A puff model is used for instantaneous or near-instantaneous releases (Hanna, 1996a). For a puff, longitudinal dispersion also occurs.

$$\chi(x,y,z;t) = \frac{Q_T}{(2\pi)^{3/2}\,\sigma_x\sigma_y\,\sigma_z}\exp\left[-\frac{1}{2}\left(\frac{x-x_o}{\sigma_x}\right)^2\right]\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \tag{A-4}$$

where:

Q_T = total source term [mg] for chemical releases

σ_x = longitudinal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the downwind axis direction [m]

x_o = $u \times t$; representing center of the puff in the longitudinal direction [m]

It is common practice to set σ_x equal to σ_y and to use the plume dispersion parameters[37] (Hanna, 1996a).

[37] The dispersion parameters for a puff release are known to be different than those for a plume release. Most dispersion models use plume dispersion parameters for both puff and plume releases due to the more extensive data available for plume releases (Hanna, 1996a).

ALOHA Application of Gaussian Dispersion Models

For direct source releases and pipe source releases in which the pipe is connected to a large-capacity reservoir, the airborne release rate remains steady. ALOHA calculates time-dependent airborne release rates for the other source cases. Recall that ALOHA calculates instantaneous release rates for up to 150 time steps. ALOHA then averages the release rates from the individual time steps over five averaging periods at most.[38] The five averaging periods are selected to most accurately portray the peak emissions. The five average release rates and associated duration for each (i.e., averaging periods) are inputs to the ALOHA algorithms for atmospheric transport and dispersion. ALOHA tracks the evolution of the mean concentration field of the five separate chemical clouds and calculates the concentration at a given time and location through superimposition.

ALOHA uses algebraic expressions for σ_y and σ_z that are a function of x and based on established σ_y and σ_z curves (based on data from field experiments). Recall that each σ_y or σ_z curve (and associated algebraic expression) reflects a specific atmospheric stability class and ground roughness condition (typically identified as either rural or urban[39]). Briggs developed the algebraic expressions that are incorporated into ALOHA. Briggs used a set of σ_y curves that reflect a 3-minute averaging time based on Prairie grass data.[40] ALOHA does not adjust σ_y for plume meander due to a different averaging time for the release. Following convention, σ_x is set equal to σ_y. Two sets of σ_z curves are used by ALOHA for rural and urban environments, respectively. The rural σ_z values reflect an averaging time of 10 to 15 minutes, and the urban σ_z values reflect a 1-hour averaging time (Reynolds, 1992).

Documentation for ALOHA suggests that it uses the wind speed at the height of 10 meters for the average wind speed in the Gaussian dispersion models for puffs and plumes (Reynolds, 1992).

DENSE GAS MODEL

A dense-gas cloud that is released to the atmosphere resists the influences of the hydraulic pressure field associated with the atmospheric wind and deflects the atmospheric wind around the cloud. Mixing occurs at the edges of the cloud. Unlike the Gaussian models used by the ALOHA code for neutrally buoyant transport and dispersion, the dense-gas set of equations used

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[38] One minute is the minimum duration for an averaging period, so the number of averaging periods is less than five when the total release duration is less than five minutes.

[39] ALOHA uses the phrase "open country" in place of "rural" and "urban and forest" in place of "urban".

[40] Following a recommendation by the ALOHA Review Committee, the σ_y curves that were developed by Briggs for the urban environment were not used. Instead, the σ_y curves that were developed for rural environments (i.e, Prairie Grass data) are conservatively used for both rural and urban applications (Reynolds, 1992).

by ALOHA is too complicated to be presented and discussed in a condensed manner.[41] As a result, the approach taken in this report is to briefly highlight important phenomena associated with dense-gas transport and dispersion and summarize the historical background of the algorithms (Reynolds, 1992).

Initially, the cloud hugs the ground under the influence of its high density and spreads laterally similar to that of a liquid spill. The density distribution in the vertical direction of the slumping cloud is stably stratified, which inhibits turbulence and entrainment of air at the top of the cloud.[42] Dense-gas cloud dispersion is thus characterized by significantly greater lateral (crosswind) spreading and reduced vertical spreading as compared to the spreading that occurs with a neutrally buoyant release. As the cloud travels downwind, enough air is entrained into the cloud that cloud density approaches that of the ambient air. The atmospheric transport and dispersion of the cloud then takes on the characteristics of that of a neutrally buoyant cloud. For small releases, this may take place as close as a few meters from the source (NOAA, 1999a).

The dense-gas dispersion model used by ALOHA is a simplified version of the DEGADIS dense-gas dispersion model (Havens, 1985; Spicer 1989). DEGADIS itself is an adaptation of the HEGADIS model that was developed by Shell Research (Colenbrander, 1980; Colenbrander, 1983). The ALOHA-DEGADIS algorithm incorporates simplifications that lessen input data needs and speed up computations (Reynolds, 1992). The ALOHA-DEGADIS model uses dispersion coefficients that are based on a five-minute averaging time. Benchmark tests show that the ALOHA-DEGADIS algorithm produces slightly conservative results (on the order of 10% higher peak concentrations) in comparison with DEGADIS results (Reynolds, 1992).

[41] The draft technical memorandum documents the 14 equations that ALOHA solves simultaneously to arrive at a solution for downwind concentration (Reynolds, 1992).

[42] If the temperature of the ground or air is higher than cloud, positive heat flow results, which reduces the cloud stability.

APPENDIX B: TORNADO DILUTION FACTOR

Atmospheric transport and dispersion of chemical material from the facility into the environment during a tornado can be modeled with a design basis accident dilution factor (Ψ/Q) designated for a specific class tornado and applied for the distance from the facility to the receptor. The Ψ/Q parameter (units of s/m^3) represents the time-integrated ground-level centerline air concentration normalized by the mass released and is analogous to the χ/Q value that is calculated from the Gaussian plume equation for neutrally buoyant releases as discussed in Appendix A. The Fujita scale is commonly used to categorize tornadoes. For most safety analysis applications, the tornado is assumed to be either Fujita - 2 (F2) or F3. Figure B-1 shows Ψ/Q values (s/m^3) as a function of downwind distance (km) for different mean translational speeds of the F2 tornado (Weber and Hunter, 1996). The consequence analysis should pick a maximum Ψ/Q for the assumed translational speed. For example, the translational speed of 7.5 m/s leads to a maximum air concentration at approximately three kilometers. The product of thus maximum Ψ/Q value with the release rate of the chemical to the atmosphere yields the ground-level air concentration at the location of interest.

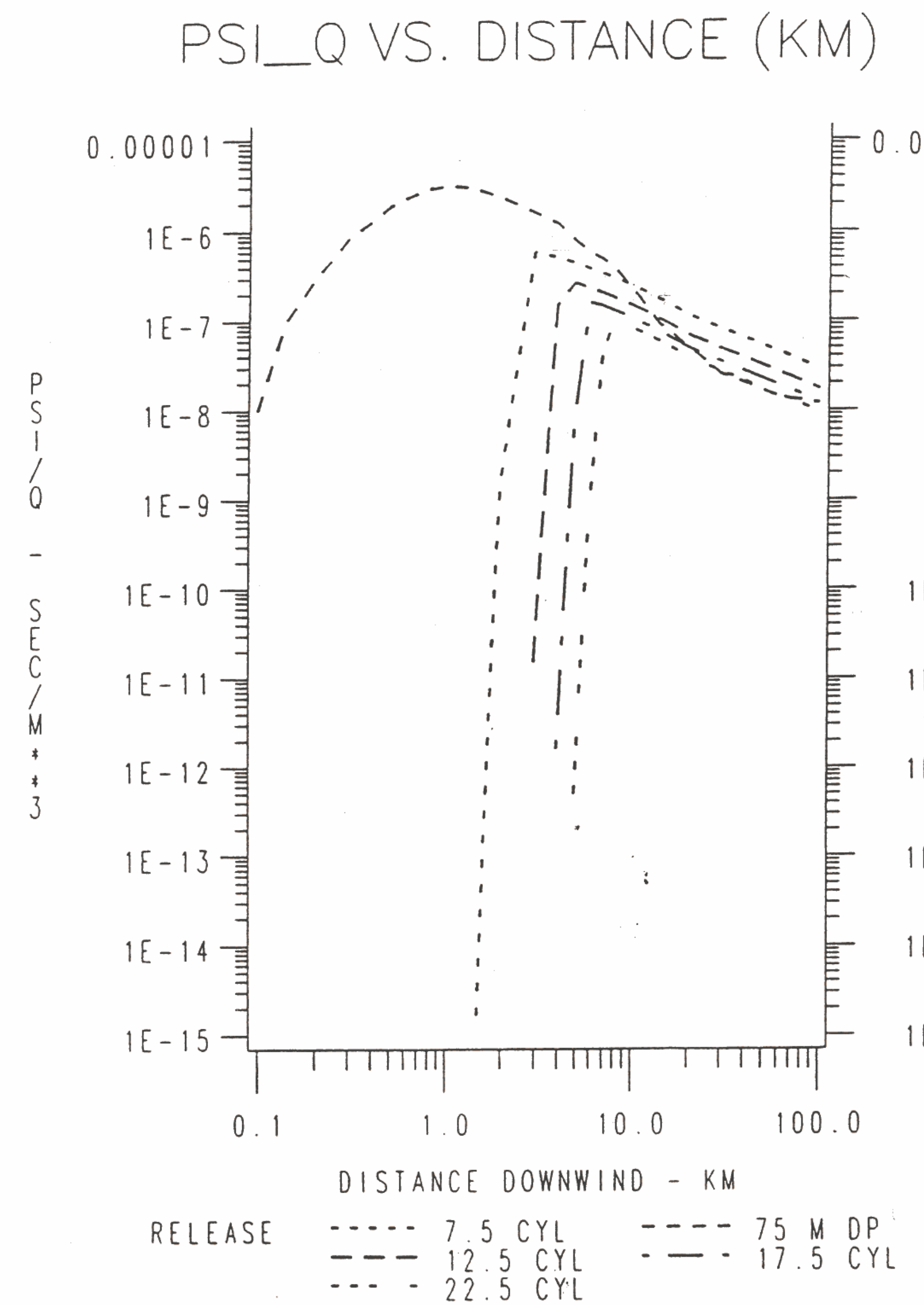

Figure B-1. The maximum time-integrated ground-level centerline air concentration (s/m^3) versus downwind distance (km) for different mean translational speeds from 7.5m/s to 22.5 m/s. The downdraft speed is 10 m/s and the height of the cylindrical mesocyclone is 3500 m (from Weber and Hunter, 1996).

APPENDIX C: DEVELOPMENTAL HISTORY OF ALOHA

(from http://response.restoration.noaa.gov/cameo/alohafaq/history.html)

NOAA OR&R Home / Chemical Aids / CAMEO Toolkit / ALOHA History

ALOHA: An Evolutionary History

Over the years, ALOHA has changed and evolved. Here's a list of the most significant modifications to the program, from most to least recent:

ALOHA 5.2.3 (Summer 1999)

- ChemManager has been eliminated; changes to the chemical library now can be made from within ALOHA.
- Direct Source allows you to more easily model venting of an indoor puddle (by allowing you to enter release rate of an evaporating vapor at ambient pressure in volume units).
- ALOHA save files are now cross platform (files saved on a Macintosh can be used in Windows, and vice versa).
- A Fat Binary version was created for Macintosh users; there is no longer a math coprocessor version.
- The chemical library has been expanded, and a few chemicals have been removed.
- ALOHA now predicts the magnitude of the initial drop in release rate from ruptured pipes connected to large reservoirs.
- Bugs found in earlier versions were fixed.
- DIPPR physical property values have been hidden from view, by request from DIPPR developers.

ALOHA 5.2.2 (Fall 1997)

- A problem in ALOHA 5.2.1 that prevented ALOHA from receiving SAM station data was corrected.

ALOHA 5.2.1 (Winter 1996)

- An erroneous value used in ALOHA 5.2 for the surface tension of ammonia was corrected. (The error caused overestimation of the rate of release of ammonia from a pressurized tank.)
- ALOHA was modified to correctly access weather data from a portable meteorological station when the data are "noisy" (noise in radio-transmitted data typically results from static caused by other electronic signals).
- The algorithm for predicting two-phase flow from a tank was refined.
- Tank and Puddle dialog boxes were modified to allow diked area to be specified as area or diameter.
- Additional LOC units options were added.
- ALOHA for Windows was modified so that it could open save files created in ALOHA 5.1 for Window.
- ALOHA for Windows was corrected to automatically load a chemical when you opened a record for a synonym for that chemical's name in CAMEO and then navigated to ALOHA.

ALOHA 5.2 (Fall 1995)

- ALOHA's heavy gas module was revised so that the heavy gas footprint is always ALOHA's best guess, rather than an overestimate. Previous versions overestimated heavy gas footprints for pressurized and/or short-duration releases.
- The Direct Source module was modified to allow you to choose the duration of a continuous release, if it lasts for more than 1 minute and less than 1 hour.
- ALOHA was modified to automatically pick a stability class, once you have entered values for wind speed, cloud cover, and time of day; you no longer need to choose the class.
- ALOHA was modified to require the wind speed measurement height, and to adjust its computations accordingly. Previous versions expected wind speed to have been measured at a height of about 3 meters (about 10 feet).

- A horizontal line representing your Level of Concern (LOC) was added to the Concentration graph.

- BitPlot was replaced by MARPLOT for Windows.

- ALOHA's online helps, alerts and dialog boxes, and manual were extensively revised.

- New physical property information replaced older information in ALOHA's chemical library. A few chemicals were removed from the library, and new chemicals were added.

- Some of ALOHA's computations were refined as a result of testing. In particular, the equations used to predict puddle evaporation, two-phase flow, and heavy gas dispersion were modified.

- Bugs found in ALOHA 5.1 were fixed.

ALOHA 5.1 (Fall 1992)

- The first Windows version of ALOHA was released.

- Complex mapping functions were moved out of ALOHA into the new mapping program, MARPLOT.

- Footprints drawn on maps were modified to appear transparent rather than opaque.

- Carcinogen warnings were added to the chemical library.

- ALOHA's values for TLV-TWAs and IDLHs were updated to the latest published values.

- AlohaSpy was included, allowing you to archive ALOHA results.

- ALOHA's online helps, alert messages, and manual were revised and updated.

- ALOHA's equation describing subsonic flow of pure gas from a ruptured tank was revised.

- A problem with a few incorrect IDLH and/or TLV values in the chemical library was corrected.

- Internal checks were added, so that a physical property is estimated via a DIPPR equation only if temperature lies within the acceptable range (if temperature is above the range, the property value given for the maximum temperature is used, and if below the range, the value for the minimum temperature is used). Previously, checks were made only for negative values of a chemical property.

- The Heavy Gas module was modified to better interpolate between points where concentration is estimated.
- ALOHA was modified to recompute the footprint whenever building type or the dose exponent is changed.
- In the Display menu, the Concentration and Dose menu options were separated from each other.
- The "Conc & Dose" dialog box was modified to allow you to specify a location in either wind-relative or absolute coordinates.
- Internal memory management was improved. In particular, index files were added to speed access to ChemLib and CityLib.
- ALOHA's checks for inappropriate combinations of wind speed, cloud cover, and stability class were refined.

ALOHA 5.05 (Fall 1991)

- An ALOHA bug was repaired, allowing you to add cities in Arizona, Idaho, New Hampshire, New Mexico, Tennessee, Guam, and Wake Island to the location library.
- ALOHA was corrected to allow it to receive data transmitted from Weatherpak portable meteorological stations.
- ALOHA was modified to better load and handle large map files.
- ALOHA was corrected to accurately predict the rate of outflow through a large hole in a tank bottom.

ALOHA 5.0 (Fall 1990)

- ALOHA was rewritten in C.
- Time-dependent Gaussian and heavy gas dispersion algorithms were added.
- Source strength algorithms were added to predict releases from leaking tanks and ruptured gas pipelines.

- ALOHA was upgraded to predict infiltration of pollutant gases into buildings.

ALOHA 4.x and Earlier Versions

ALOHA was first written in Basic for the Apple II+ in the early 1980s as a passive gas plume model for in-house use by NOAA during emergency responses. It was rewritten in FORTRAN for the Apple Macintosh in the mid-1980s. A chemical property library, meteorological station serial port interface, and base-mapping were added at that time, and an energy-balance pool evaporation algorithm was added in the late 1980s.

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Office of Response and Restoration, National Ocean Service, National Oceanic and Atmospheric Administration